

06 - 96 - 00 PCT/ **526 Rec'd PCT/TTT 23 JUN 2000**

(REV 11-98) U.S. DEPARTMENT OF COMMERCE	ATTORNEY'S DOCKET NUMBER									
TRANSMITTAL LETTER T	P02005US0									
DESIGNATED/ELECTEI	U.S. APPLICATION NO. (If known, see 37 CFR 1.5)									
CONCERNING A FILING	09/582486									
INTERNATIONAL APPLICATION NO.	INTERNATIONAL FILING DATES	PRIORITY DATE CLAIMED								
PCT/GB98/03860	24 December 1998	24 December 1997 24 June 1998								
TITLE OF INVENTION MODIFIED D	C SYNTHASE (DAOCS) AND									
X-RAY STRU APPLICANT(S) Christopher		aldwin; Peter L. Roach; Matthew D.								
FOR DO/EO/US Lloyd; Karl H	arlos; Inger Andersson; Janos Ha	ajdu; Anke S. Terwisscha Van								
	Karin Valegard; and S. Ramaswar ates Designated/Elected Office (DO/FO/I	ny JS) the following items and other information:								
[· · ·	items concerning a filing under 35 U	· -								
	QUENT submission of items concern									
		U.S.C. 371 (f)) at any time rather than								
		et in 35 U.S.C. 371 (b) and PCT Articles								
4. X A proper Demand for International Claimed.	onal Preliminary Examination was m	ade by the 19 th month from the earliest								
l —	plication as filed (35 U.S.C. 371 (c)(2))								
a. X is transmitted herewith (red	a. X is transmitted herewith (required only if not transmitted by the International Bureau).									
b. has been transmitted by th	b. has been transmitted by the International Bureau.									
c. is not required, as the appl	lication was filed in the United States	Receiving Office (RO/US).								
6. A translation of the Internation	al Application into English (35 U.S.C	. 371 (c)(2)).								
7. X Amendments to the claims of	7. X Amendments to the claims of the International Application under PCT Article 19 (35 U.S.C. 371 (c)(3))									
a. are transmitted herewith (r	equired only if not transmitted by the	International Bureau).								
b. have been transmitted by t	he International Bureau.									
c. have not been made; howe	c. have not been made; however, the time limit for making such amendments has NOT expired.									
d. X have not been made and v	d. X have not been made and will not be made.									
8. A translation of the amendmen	nts to the claims under PCT Article 1	9 (35 U.S.C. 371 (c)(3)).								
9. An oath or declaration of the inventor(s) (35 U.S.C. 371 (c)(4)).										
10. A translation of the annexes to U.S.C. 371 (c)(5)).	the International Preliminary Exami	nation Report under PCT Article 36 (35								
Items 11. to 16. below concern docu	ment(s) or information included:									
11. X An Information Disclosure Sta	tement under 37 CFR 1.97 and 1.98.									
12. An assignment document for r is included.	recording. A separate cover sheet in	compliance with 37 CFR 3.28 & 3.31								
13. X A FIRST preliminary amendme	ent.									
A SECOND or SUBSEQUENT	Fpreliminary amendment.									
14. A substitute specification.										
15. X A change of power of attorney	and/or address letter.									
16. X Other items or information: S	equence Listing and Diskette									

U.S. APPLICATION NO. (if known, see & OFR 1.	5) INTERNATIONAL AF PCT/GB98	ATTORNEY'S DOCKET NUMBER P02005US0						
17. X The following	ng fees are submitte		CALCULATIONS PTO USE ONLY						
BASIC NA Neither internation international searce and International prelin USPTO but International prelin but international prelin but all claims did r International prelin and all claims satis									
ENTER A	APPROPRIATE BA	ASIC FEE AMOUNT	· =	\$970.00					
Surcharge of		g the oath or declarat							
20 30 mont	ns from the earliest cla	aimed priority date (37	CFR 1.492 (e)).						
CLAIMS	NUMBER FILED	NUMBER EXTRA	RATE						
Total claims	232 - 20 =	212	X 18	3,816.00					
Independent claims	13 -3=	10	x 78	780.00					
MULTIPLE DEPENDE			x	-0-					
		OF ABOVE CALC		5,566.00					
Reduction of ½ for filing Statement must also be	ig by small entity, if a se filed (Note 37 CFF	pplicable. Verified Sr 2 1 9 1 27 1 28)	nall Entity						
Otatomont made also b	10 mod (11010 01 01 1		SUBTOTAL =	5,566.00					
Processing fee of	slation later than								
I — —	R 1.492 (f)). +								
	5,566.00								
Fee for recording the emust be accompanied (per pr									
	NCLOSED =	\$5,566.00							
		Refunded							
			Charged						
a. A check in the amount of to cover the above fees is enclosed.									
b. X Please charg	ge my Deposit Accou	nt No. 06-2375	in the amoun	t of \$5,566.00	į.				
to cover the above fees. A duplicate copy of this sheet is enclosed.									
c. X The Commissioner is hereby authorized to charge any additional fees which may be required or credit									
any overpayment to my Deposit Account No. 06-2375 . A duplicate copy of this sheet is enclosed.									
NOTE: Where an appropriate time limit under 37 CFR 1.494 has not been met, a petition to revive (37 CFR 1.137 (a) or (b)) must be filed and granted to restore the application to pending status.									
SEND ALL CORRESPONDENCE TO:									
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1301 McKinney, Suite 5100 Houston, TX 77010-3095 46,089									
REGISTRATION NUMBER									
6-23-	00								

09/582486 532 Rec'd PCT/PTC 23 JUN 2000

IN THE UNITED STATES PATENT AND TRADEMARK OFFICE

Serial No.: To be assigned \$ Docket No.: P02005US0 \$ Filing Date: June 16, 2000 \$ \$ Applicants: C. Schofield et al. \$ \$ Title: Modified Deacetoxycephalosporin C \$ Synthase (DAOCS) and X-Ray Structure \$

Assistant Commissioner for Patents Washington, D.C. 20231

Dear Sir:

Applicants respectfully request the entry of the present statement in regard to the enclosed sequence listing in the above-referenced application. The submitted materials include a computer readable form and paper copy of a sequence listing for the sequence found in the application (SEQ ID NO: 1). Applicants state the information recorded in the computer readable form of the sequence listing is identical to the written sequence listing. Applicants also state that the submission, filed in accordance with 37 CFR 1.821(g), does not include new matter. The sequence found in the sequence listing is identical to that found in the application.

If you have any questions regarding the above-referenced application, please do not hesitate to contact me.

Respectfully submitted,

Melissa D. Schwaller, Ph.D.

Melissa D. Schwaller

Registration No. 46,089

Date: 6-23-00

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SEQUENCE LISTING

<110> SCHOFIELD, Christopher J.
 BALDWIN, Jack E.
 LLOYD, Matthew D.
 HARLOS, Karl
 ANDERSSON, Inger
 TERWISSCHA VAN SCHELTINGA, Anke S.
 VALEGARD, Karin
 RAMASWAMY, S.

<120> MODIFIED DEACETOXYCEPHALOSPORIN C SYNTHASE (DAOCS) AND X-RAY STRUCTURE

<130> 08004624

<140> PCT/GB98/03860

<141> 1998-12-24

<150> 9727370.0

<151> 1997-12-24

<150> 9813644.3

<151> 1998-06-24

<160> 1

<170> PatentIn Ver. 2.1

<210> 1

<211> 311

<212> PRT

<213> Streptomyces clavuligerus

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Ala Val Thr Ser Pro Val Pro Thr Met Arg Arg Gly Phe Thr Gly Leu

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Gly	Asp	Phe 115	Gly	Arg	Ile	Trp	Thr 120	Gln	Tyr	Phe	Asp	Arg 125	Gln	Tyr	Thr
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Pro 145	Asp	Gly	Gly	Val	Glu 150	Ala	Phe	Leu	Asp	Cys 155	Glu	Pro	Leu	Leu	Arg 160
Phe	Arg	Tyr	Phe	Pro 165	Gln	Val	Pro	Glu	His 170	Arg	Ser	Ala	Glu	Glu 175	Gln
Pro	Leu	Arg	Met 180	Ala	Pro	His	Tyr	Asp 185	Leu	Ser	Met	Val	Thr 190	Leu	Ile
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Ile Arg Arg Thr Ser Lys Ala 305 310

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IN THE UNITED STATES PATENT AND TRADEMARK OFFICE

APPLICANT:

C. J. SCHOFIELD ET AL.

DOCKET NO.

P02005US0

FILING DATE:

TO BE ASSIGNED

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SERIAL NO.:

TO BE ASSIGNED

Gr : To be

assigned

TITLE:

MODIFIED DEACETOXYCEPHALOSPORIN:

C SYNTHASE (DAOCS) AND X-RAY

Examiner:

STRUCTURE

To be assigned

Assistant Commissioner of Patents

Washington, D.C. 20231

FIRST PRELIMINARY AMENDMENT

Dear Sir:

Please enter the following amendments to the claims prior to the examination of the application.

IN THE CLAIMS:

Please amend the claims as follows:

- 1. (amended) Deacetoxycephaloporin C synthase (DAOCS) having a structure designated by the X-ray co-ordinates of structure A or structure B [herein].
- 2. (amended) DAOCS in the form of a complex with a metal, [e.g. iron or lead, and optionally in the presence of a substrate and/or a substrate analogue or inhibitor,] having a structure designated by the X-ray co-ordinates [herein] of structure B.
- 3. (amended) DAOCS as claimed in claim [2] <u>28</u>, wherein the substrate is <u>selected from the group consisting of penicillin N, penicillin G, 2-oxoglutarate or dioxygen [,and the inhibitor is selected from N-oxalylamino acids, pyridine-carboxylates and nitrous oxide].</u>
- 4. (amended) [Use of the three-dimensional structure of DAOCS for the modification of] A method of modifying DAOCS or other related 2-oxoglutarate dependent [enzyme] enzymes comprising referring to the three-dimensional structure of DAOCS to select the modification of said enzymes.
- 5. (amended) [Use as claimed in] The method of claim 4, wherein the related 2-oxoglutarate dependent enzyme is DACS, DAOC/DACS or the oxygenase enzyme involved in the introduction of the 7α -methoxy group into cephamycin C.
- 6. (amended) [Use as claimed in] The method of claim 5, [for] wherein the modification of DAOCS, DACS or DAOC/DACS is such that they accept unnatural substrates more efficiently than the wild type enzymes.

- 7. (amended) [Use as claimed in] The method of claim 5, [for] wherein the modification of DAOCS, DACS, DAOC/DACS is such that they convert natural substrates to pharmaceuticals or useful intermediates in the preparation of pharmaceuticals.
- 8. (amended) [Use as claimed in] The method of claim 6, wherein the unnatural substrates are penicillins [including penicillin G, penicillin V, 6-aminopenicillanic acid, amoxycillin, or penicillins with a phenyl glycine or p-hydroxyphenyl glycine side chain].
- 9. (amended) [Use as claimed in] The method of claim 6, wherein the unnatural substrate is a cephalosporin.
- 10. (amended) [Use as claimed in] The method of claim 6, wherein the unnatural substrate is an amino acid or a peptide.
- 11. (amended) [Use as claimed in any one of claims] The method of claim 6[-8], wherein [penicillin G, penicillin V, another] unnatural substrate [or penicillin N] is converted to a cephalosporin [or exomethylene cephalosporin].
- 12. (amended) An enzyme having significant [(as herein defined)] sequence similarity to DAOCS, wherein the side chain binding site of [penicillin N or] DAOC is modified and at least one amino acid residue [and] at [at least] one or more of the following sites [at least one amino acid residue] selected from the group consisting of Thr72, Arg74, Arg75, Glu156, Leu158, Arg160, Arg162, Leu186, Ser187, Phe225, Phe264, Arg266, Asp301, Tyr302, Val303, and Asn304; is changed to another amino acid residue or is deleted[: Thr72, Arg74, Arg75, Glu156, Leu158, Arg160, Arg162, Leu186, Ser187, Phe225, Phe264, Arg266, Asp301, Tyr302, Val303, Leu158, Arg160, Arg162, Leu186, Ser187, Phe225, Phe264, Arg266, Asp301, Tyr302, Val303,

and Asn304; and/or at least one additional amino acid residue is inserted within the region 300-311; provided that other residues interacting with the above may be changed in order to accommodate the change in one of the above].

- 13. (amended) An enzyme having significant [(as herein defined)] sequence similarity to DAOCS, wherein the penicillin/cephalosporin binding site of [penicillin N or] DAOC is modified [and at] at [least] one or more of the following amino acid residues selected from the group consisting of Ile 88, Arg160, Arg162, Phe164, Met180, Thr190, Ile192, Phe225, Pro241, Val245, Val262, Phe264, Ile305, Arg 306, and Arg307; is changed or deleted: [Ile 88, Arg160, Arg162, Phe164, Met180, Thr190, Ile192, Phe225, Pro241, Val245, Val262, Phe264, Ile305, Arg 306, and Arg307; and/or at least one additional amino acid residue is inserted within the region 300-311; provided that other residues interacting with the above may be changed in order to accommodate the change in one of the above].
- 14. (amended) An enzyme according to claim 12 [or claim 13] which is a [mutant] modification of DAOCS or DACS or DAOC/DACS.
- 15. (amended) An enzyme [as claimed in any one of claims 12-14] having significant sequence similarity to DAOCS, wherein both the side chain and the penicillin/cephalosporin binding sites of penicillin N or DAOC are modified and at least one of the residues [specified in claims 12 and 13] selected from the group consisting of Thr72, Arg74, Arg75, Ile88, Glu156, Leu158, Arg160, Arg162, Phe164, Met180, Leu186, Ser187, Thr190, Ile192, Phe225, Pro241, Val245, Val262, Phe264, Arg266, Asp301, Tyr302, Val303, Asn304; Ile305, Arg 306, and Arg307 is changed or deleted [and/or at least one additional amino acid residue is inserted within the region 300-311; provided that other residues interacting with the above may be changed in order to accommodate the change in one of the above].

- 16. (amended) An enzyme as claimed in [any one of claims] <u>claim</u> 12[-15], wherein two or more complementary mutations are introduced to create or delete a binding interaction, including H-bonds, electrostatic, or hydrophobic interactions.
- 17. (amended) A [gene] polynucleotide encoding [for] the enzyme of [any one of claims] claim 12[-16].
- 18. (amended) A micro-organism capable of expressing the [gene] polynucleotide of claim 17 under fermentation conditions.
- 19. (amended) [Use of] The method of using the micro-organisms of claim 18 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.
- 20. (amended) [Use as claimed in] The method of claim 19, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway [including isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase].
- 22. (amended) A method as claimed in claim 21 wherein the said other related 2-osoglutarate dependent enzyme or related enzyme is 1-aminocylopropane-1-carboxylate oxidase, gibberellin C-20 oxidase, flavone synthase, flavanone 3β -hydroxylase, hyoscyamine 6β -hydroxylase, prolyl 4-hydroxylase, prolyl 3-hydroxylase, aspartyl hydroxylase, lysyl hydroxylase, proline hydroxylases, γ -butyrobetaine hydroxylase, enzymes in herbicide resistance mechanisms, clavaminate synthase, and oxygenase enzyme involved in the biosynthesis of carbapenems, the [so called] ethylene forming enzyme from *Pseudomonas syringe*, p-

hydroxyphenylpyruvate dioxgenase, [and] <u>or</u> an oxygenase enzyme involved in the oxidation of phytol in human liver peroxisomes.

- 23. (amended) A method as claimed in claim 21 [or 22] wherein the said other enzyme is modified, by deletion or addition or alteration; at one or more of the sites [defined in claim 12 or 13] selected from the group consisting of Thr72, Arg74, Arg75, Ile 88, Glu156, Leu158, Arg160, Arg162, Phe164, Met180, Leu186, Ser187, Thr190, Ile192, Phe225, Pro241, Val245, Val262, Phe264, Arg266, Asp301, Tyr302, Val303, Asn304; Ile305, Arg 306, and Arg307; or using the following information for the design [or] of an inhibitor: Asp185, His183 and His243 act as ligand to the iron; Arg258 and Ser260 and the Fe bind the 2-oxoglutarate; Met180, Phe225, Leu31 and Val245 are close to the iron binding site; Tyr33, Arg160, Arg162, Phe164, Ile192, Gln194, Leu204, Leu223, Leu215 are important for the construction of the part of the active site binding 2-oxoglutarate; and Arg160 and Arg162 are important for binding an amino acid or peptide derived substrate.
- 24. (amended) A method as claimed in [any one of claims] <u>claim</u> 21[-23], wherein the said other enzyme is prolyl 4-hydroxylase, prolyl 3-hydroxylase, aspartyl hydroxylase, or lysyl hydroxylase and the inhibitor is to be used for the treatment of human diseases including fibrotic diseases including liver cirrhosis and arthritis.
- 25. (amended) A method as claimed in [any one of claims] <u>claim</u> 21[-23], wherein the said other enzyme is p-hydroxyphenylpyruvate dioxygenase and the inhibitor is to be used in the treatment of certain genetic disorders.
- 26. (amended) A method as claimed in [any one of claims] <u>claim</u> 21[-23], wherein the said other enzyme is involved in herbicide resistance and the information is to be used to design new herbicides to overcome the problem of resistance.

Please add the following new claims:

- 27. The DAOCS of claim 2, wherein said metal is iron or lead.
- 28. The DAOCS of claim 2, wherein said complex includes a substrate.
- 29. The DAOCS of claim 2, wherein said complex includes a substrate analogue.
- 30. The DAOCS of claim 2, wherein said complex includes an inhibitor.
- 31. DAOCS as claimed in claim 30, wherein the inhibitor is selected from the group consisting of N-oxalylamino acids, pyridine-carboxylates and nitrous oxide.
- 32. The method of claim 8, wherein said penicillins are selected from the group consisting of penicillin G, penicillin V, 6-aminopenicillanic acid, amoxycillin, and penicillins with a phenyl glycine or p-hydroxyphenyl glycine side chain.
- 33. The method of claim 10, wherein said amino acid is a proteinogenic amino acid.

- 34. (amended) [Use as claimed in any one of claims] The method of claim 6[-8], wherein [penicillin G, penicillin V, another] unnatural substrate [or penicillin N] is converted to a [cephalosporin or] exomethylene cephalosporin.
- 35. The method of claim 8, wherein penicillin G, penicillin V or penicillin N is converted to a cephalosporin.
- 36. The method of claim 8, wherein penicillin G, penicillin V or penicillin N is converted to an exomethylene cephalosporin.
- 37. The enzyme of claim 12, further comprising the insertion of at least one additional amino acid residue within the region 300-311.
- 38. An enzyme having significant sequence similarity to DAOCS, wherein the side chain binding site of DAOC is modified and at least one additional amino acid residue is inserted within the region 300-311.
- 39. An enzyme having significant sequence similarity to DAOCS, wherein the side chain binding site of DAOC is modified and at least one amino acid residue at one or more of the following sites selected from the group consisting of Thr72, Arg74, Arg75, Glu156, Leu158, Arg160, Arg162, Leu186, Ser187, Phe225, Phe264, Arg266, Asp301, Tyr302, Val303, and Asn304; is changed to another amino acid residue or is deleted.

- 40. The enzyme of claim 12, further comprising the insertion of at least one additional amino acid residue within the region 300-311.
- 41. An enzyme having significant sequence similarity to DAOCS, wherein the side chain binding site of penicillin N is modified and at least one additional amino acid residue is inserted within the region 300-311.
- 42. The enzyme of claim 13, further comprising the insertion of at least one additional amino acid residue within the region 300-311.
- 43. An enzyme having significant sequence similarity to DAOCS, wherein the penicillin/cephalosporin binding site of DAOC is modified and at least one additional amino acid residue is inserted within the region 300-311.
- 44. An enzyme having significant sequence similarity to DAOCS, wherein the penicillin/cephalosporin binding site of penicillin N is modified at one or more of the following amino acid residues selected from the group consisting of Ile 88, Arg160, Arg162, Phe164, Met180, Thr190, Ile192, Phe225, Pro241, Val245, Val262, Phe264, Ile305, Arg 306, and Arg307; is changed or deleted.
- 45. The enzyme of claim 13, further comprising the insertion of at least one additional amino acid residue within the region 300-311.

- 46. An enzyme having significant sequence similarity to DAOCS, wherein the penicillin/cephalosporin binding site of DAOC is modified and at least one additional amino acid residue is inserted within the region 300-311.
- 47. The enzyme of claim 15, further comprising the insertion of at least one additional amino acid residue within the region 300-311.
- 48. An enzyme having significant sequence similarity to DAOCS, wherein both side chain and the penicillin/cephalosporin binding site of DAOC are modified and at least one additional amino acid residue is inserted within the region 300-311.
- 49. An enzyme according to claim 13 which is a modification of DAOCS or DACS or DAOC/DACS.
- 50. An enzyme according to claim 15 which is a modification of DAOCS or DACS or DAOC/DACS.
- 51. An enzyme as claimed in claim 13, wherein two or more complementary mutations are introduced to create or delete a binding interaction, including H-bonds, electrostatic, or hydrophobic interactions.
- 52. An enzyme as claimed in claim 14, wherein two or more complementary mutations are introduced to create or delete a binding interaction, including H-bonds, electrostatic, or hydrophobic interactions.

- 53. An enzyme as claimed in claim 49, wherein two or more complementary mutations are introduced to create or delete a binding interaction, including H-bonds, electrostatic, or hydrophobic interactions.
- 54. An enzyme as claimed in claim 15, wherein two or more complementary mutations are introduced to create or delete a binding interaction, including H-bonds, electrostatic, or hydrophobic interactions.
- 55. An enzyme as claimed in claim 37, wherein two or more complementary mutations are introduced to create or delete a binding interaction, including H-bonds, electrostatic, or hydrophobic interactions.
- 56. An enzyme as claimed in claim 38, wherein two or more complementary mutations are introduced to create or delete a binding interaction, including H-bonds, electrostatic, or hydrophobic interactions.
- 57. An enzyme as claimed in claim 39, wherein two or more complementary mutations are introduced to create or delete a binding interaction, including H-bonds, electrostatic, or hydrophobic interactions.
- 58. An enzyme as claimed in claim 40, wherein two or more complementary mutations are introduced to create or delete a binding interaction, including H-bonds, electrostatic, or hydrophobic interactions.

- 59. An enzyme as claimed in claim 41, wherein two or more complementary mutations are introduced to create or delete a binding interaction, including H-bonds, electrostatic, or hydrophobic interactions.
- 60. An enzyme as claimed in claim 42, wherein two or more complementary mutations are introduced to create or delete a binding interaction, including H-bonds, electrostatic, or hydrophobic interactions.
- 61. An enzyme as claimed in claim 43, wherein two or more complementary mutations are introduced to create or delete a binding interaction, including H-bonds, electrostatic, or hydrophobic interactions.
- 62. An enzyme as claimed in claim 44, wherein two or more complementary mutations are introduced to create or delete a binding interaction, including H-bonds, electrostatic, or hydrophobic interactions.
- 63. An enzyme as claimed in claim 45, wherein two or more complementary mutations are introduced to create or delete a binding interaction, including H-bonds, electrostatic, or hydrophobic interactions.
- 64. An enzyme as claimed in claim 46, wherein two or more complementary mutations are introduced to create or delete a binding interaction, including H-bonds, electrostatic, or hydrophobic interactions.

- 65. An enzyme as claimed in claim 47, wherein two or more complementary mutations are introduced to create or delete a binding interaction, including H-bonds, electrostatic, or hydrophobic interactions.
- 66. An enzyme as claimed in claim 48, wherein two or more complementary mutations are introduced to create or delete a binding interaction, including H-bonds, electrostatic, or hydrophobic interactions.
- 67. A polynucleotide encoding for the enzyme of claim 13.
- 68. A polynucleotide encoding for the enzyme of claim 14.
- 69. A polynucleotide encoding for the enzyme of claim 49.
- 70. A polynucleotide encoding for the enzyme of claim 15.
- 71. A polynucleotide encoding for the enzyme of claim 16.
- 72. A polynucleotide encoding for the enzyme of claim 37.

82.

A polynucleotide encoding for the enzyme of claim 38. 73. A polynucleotide encoding for the enzyme of claim 39. 74. A polynucleotide encoding for the enzyme of claim 40. 75. A polynucleotide encoding for the enzyme of claim 41. 76. A polynucleotide encoding for the enzyme of claim 42. 77. A polynucleotide encoding for the enzyme of claim 43. A polynucleotide encoding for the enzyme of claim 44. 79. A polynucleotide encoding for the enzyme of claim 45. 80. A polynucleotide encoding for the enzyme of claim 46. 81.

A polynucleotide encoding for the enzyme of claim 47.

92.

83. A polynucleotide encoding for the enzyme of claim 48. A polynucleotide encoding for the enzyme of claim 50. 84. A polynucleotide encoding for the enzyme of claim 51. 85. A polynucleotide encoding for the enzyme of claim 52. 86. A polynucleotide encoding for the enzyme of claim 53. 87. 88. A polynucleotide encoding for the enzyme of claim 54. A polynucleotide encoding for the enzyme of claim 55. 89. A polynucleotide encoding for the enzyme of claim 56. 90. A polynucleotide encoding for the enzyme of claim 57. 91.

A polynucleotide encoding for the enzyme of claim 58.

fermentation conditions.

A polynucleotide encoding for the enzyme of claim 59. 93. A polynucleotide encoding for the enzyme of claim 60. 94. A polynucleotide encoding for the enzyme of claim 61. 95. A polynucleotide encoding for the enzyme of claim 62. 96. A polynucleotide encoding for the enzyme of claim 63. 97. A polynucleotide encoding for the enzyme of claim 64. 98. A micro-organism capable of expressing the polynucleotide of claim 67 under 99. fermentation conditions. A micro-organism capable of expressing the polynucleotide of claim 68 under 100. fermentation conditions.

A micro-organism capable of expressing the polynucleotide of claim 69 under

- 102. A micro-organism capable of expressing the polynucleotide of claim 70 under fermentation conditions.
- 103. A micro-organism capable of expressing the polynucleotide of claim 71 under fermentation conditions.
- 104. A micro-organism capable of expressing the polynucleotide of claim 72 under fermentation conditions.
- 105. A micro-organism capable of expressing the polynucleotide of claim 73 under fermentation conditions.
- 106. A micro-organism capable of expressing the polynucleotide of claim 74 under fermentation conditions.
- 107. A micro-organism capable of expressing the polynucleotide of claim 75 under fermentation conditions.
- 108. A micro-organism capable of expressing the polynucleotide of claim 76 under fermentation conditions.
- 109. A micro-organism capable of expressing the polynucleotide of claim 77 under fermentation conditions.

- 110. A micro-organism capable of expressing the polynucleotide of claim 78 under fermentation conditions.
- 111. A micro-organism capable of expressing the polynucleotide of claim 79 under fermentation conditions.
- 112. A micro-organism capable of expressing the polynucleotide of claim 80 under fermentation conditions.
- 113. A micro-organism capable of expressing the polynucleotide of claim 81 under fermentation conditions.
- 114. A micro-organism capable of expressing the polynucleotide of claim 82 under fermentation conditions.
- 115. A micro-organism capable of expressing the polynucleotide of claim 83 under fermentation conditions.
- 116. A micro-organism capable of expressing the polynucleotide of claim 84 under fermentation conditions.

- 117. A micro-organism capable of expressing the polynucleotide of claim 85 under fermentation conditions.
- 118. A micro-organism capable of expressing the polynucleotide of claim 86 under fermentation conditions.
- 119. A micro-organism capable of expressing the polynucleotide of claim 87 under fermentation conditions.
- 120. A micro-organism capable of expressing the polynucleotide of claim 88 under fermentation conditions.
- 121. A micro-organism capable of expressing the polynucleotide of claim 89 under fermentation conditions.
- 122. A micro-organism capable of expressing the polynucleotide of claim 90 under fermentation conditions.
- 123. A micro-organism capable of expressing the polynucleotide of claim 91 under fermentation conditions.
- 124. A micro-organism capable of expressing the polynucleotide of claim 92 under fermentation conditions.

- 125. A micro-organism capable of expressing the polynucleotide of claim 93 under fermentation conditions.
- 126. A micro-organism capable of expressing the polynucleotide of claim 94 under fermentation conditions.
- 127. A micro-organism capable of expressing the polynucleotide of claim 95 under fermentation conditions.
- 128. A micro-organism capable of expressing the polynucleotide of claim 96 under fermentation conditions.
- 129. A micro-organism capable of expressing the polynucleotide of claim 97 under fermentation conditions.
- 130. A micro-organism capable of expressing the polynucleotide of claim 98 under fermentation conditions.
- 131. The method of using the micro-organisms of claim 99 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.

- 132. The method of using the micro-organisms of claim 100 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.
- 133. The method of using the micro-organisms of claim 101 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.
- 134. The method of using the micro-organisms of claim 102 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.
- 135. The method of using the micro-organisms of claim 103 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.
- 136. The method of using the micro-organisms of claim 104 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.
- 137. The method of using the micro-organisms of claim 105 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.
- 138. The method of using the micro-organisms of claim 106 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.
- 139. The method of using the micro-organisms of claim 107 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.

- 140. The method of using the micro-organisms of claim 108 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.
- 141. The method of using the micro-organisms of claim 109 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.
- 142. The method of using the micro-organisms of claim 110 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.
- 143. The method of using the micro-organisms of claim 111 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.
- 144. The method of using the micro-organisms of claim 112 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.
- 145. The method of using the micro-organisms of claim 113 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.
- 146. The method of using the micro-organisms of claim 114 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.

- 147. The method of using the micro-organisms of claim 115 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.
- 148. The method of using the micro-organisms of claim 116 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.
- The method of using the micro-organisms of claim 117 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.
- 150. The method of using the micro-organisms of claim 118 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.
- 151. The method of using the micro-organisms of claim 119 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.
- 152. The method of using the micro-organisms of claim 120 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.
- 153. The method of using the micro-organisms of claim 121 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.
- 154. The method of using the micro-organisms of claim 122 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.

- 155. The method of using the micro-organisms of claim 123 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.
- 156. The method of using the micro-organisms of claim 124 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.
- 157. The method of using the micro-organisms of claim 125 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.
- 158. The method of using the micro-organisms of claim 126 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.
- 159. The method of using the micro-organisms of claim 127 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.
- 160. The method of using the micro-organisms of claim 128 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.
- 161. The method of using the micro-organisms of claim 129 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.

- 162. The method of using the micro-organisms of claim 130 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.
- 163. The method of claim 131, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.
- 164. The method of claim 132 wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.
- 165. The method of claim 133, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.
- 166. The method of claim 134, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.
- 167. The method of claim 135, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.
- 168. The method of claim 136, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.
- 169. The method of claim 137, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.

- 170. The method of claim 138, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.
- 171. The method of claim 139, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.
- 172. The method of claim 140, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.
- 173. The method of claim 141, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.
- 174. The method of claim 142, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.
- 175. The method of claim 143, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.
- 176. The method of claim 144, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.

- 177. The method of claim 145, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.
- 178. The method of claim 146, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.
- 179. The method of claim 147, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.
- 180. The method of claim 148, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.
- 181. The method of claim 149, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.
- 182. The method of claim 150, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.
- 183. The method of claim 151, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.
- 184. The method of claim 152, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.

- 185. The method of claim 153, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.
- 186. The method of claim 154, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.
- 187. The method of claim 155, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.
- 188. The method of claim 156, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.
- 189. The method of claim 157, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.
- 190. The method of claim 158, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.
- 191. The method of claim 159, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.

- 192. The method of claim 160, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.
- 193. The method of claim 161, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.
- 194. The method of claim 162, wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway.
- 195. The method of claim 163, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.
- 196. The method of claim 164, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.
- 197. The method of claim 165, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.
- 198. The method of claim 166, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.

- 199. The method of claim 167, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.
- 200. The method of claim 168, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.
- 201. The method of claim 169, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.
- 202. The method of claim 170, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.
- 203. The method of claim 171, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.
- 204. The method of claim 172, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.

- 205. The method of claim 173, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.
- 206. The method of claim 174, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.
- 207. The method of claim 175, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.
- 208. The method of claim 176, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.
- 209. The method of claim 177, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.
- 210. The method of claim 178, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.

- 211. The method of claim 179, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.
- 212. The method of claim 180, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.
- 213. The method of claim 181, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.
- 214. The method of claim 182, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.
- 215. The method of claim 183, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.
- 216. The method of claim 184, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.

- 217. The method of claim 185, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.
- 218. The method of claim 186, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.
- 219. The method of claim 187, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.
- 220. The method of claim 188, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.
- 221. The method of claim 189, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.
- 222. The method of claim 190, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.

- 223. The method of claim 191, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.
- 224. The method of claim 192, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.
- 225. The method of claim 193, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.
- 226. The method of claim 194, wherein said modified enzyme is isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.
- 227. A method as claimed in claim 22 wherein the said other enzyme is modified, by deletion or addition or alteration; at one or more of the sites selected from the group consisting of Thr72, Arg74, Arg75, Ile88, Glu156, Leu158, Arg160, Arg162, Phe164, Met180, Leu186, Ser187, Thr190, Ile192, Phe225, Pro241, Val245, Val262, Phe264, Arg266, Asp301, Tyr302, Val303, Asn304; Ile305, Arg 306, and Arg307; or using the following information for the design of an inhibitor: Asp185, His183 and His243 act as ligand to the iron; Arg258 and Ser260 and the Fe bind the 2-oxoglutarate; Met180, Phe225, Leu31 and Val245 are close to the iron binding site; Tyr33, Arg160, Arg162, Phe164, Ile192, Gln194, Leu204, Leu223, Leu215 are important for the

construction of the part of the active site binding 2-oxoglutarate; and Arg160 and Arg162 are important for binding an amino acid or peptide derived substrate.

- 228. A method as claimed in claim 23, wherein the said other enzyme is prolyl 4-hydroxylase, prolyl 3-hydroxylase, aspartyl hydroxylase, or lysyl hydroxylase and the inhibitor is to be used for the treatment of human diseases including fibrotic diseases including liver cirrhosis and arthritis.
- 229. A method as claimed in claim 23, wherein the said other enzyme is p-hydroxyphenylpyruvate dioxygenase and the inhibitor is to be used in the treatment of certain genetic disorders.
- 230. A method as claimed in claim 23, wherein the said other enzyme is involved in herbicide resistance and the information is to be used to design new herbicides to overcome the problem of resistance.
- 231. A polynucleotide encoding for the enzyme of claim 65.
- 232. A polynucleotide encoding for the enzyme of claim 66.

REMARKS

Entry of the amendments to the claims before examination of the application is respectfully requested. The claims have been amended for the sake of clarity. No new matter has been added by these amendments. Applicants authorize the Commissioner to charge any

required fees to Deposit Account No. 06-2375, from which the undersigned is authorized to draw.

Respectfully submitted,

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MODIFIED DEACETOXYCEPHALOSPORIN C SYNTHASE (DAOCS) AND X-RAY STRUCTURE

Penicillin and cephalosporin antibiotics are produced either directly by fermentation or by modification of fermentation derived materials containing a beta-lactam ring. The biosynthetic pathway to the penicillins and cephalosporins has been extensively studied and reviewed (J. E. Baldwin and C. J. Schofield, in 'The Chemistry of β-lactams (Ed. M. I. Page), Chapter 1, Blackie, London 1992; Ingolia and Queener, Med. Res. Rev., 1989, 9, 245-264; Aharonowitz, Cohen and Martin, Ann. Rev. Microbiol., 1992, 46, 461-495; Schofield, Bycroft, Baldwin, Hadju, Roach, Current Opinion in Structural Biology, 1997, 7, 857-864) and includes the following steps (Figure 1):

- Conversion of the tripeptide: <u>L</u>-δ-α-aminoadipoyl-<u>L</u>-cysteinyl-<u>D</u>-valine (ACV) to isopenicillin N in a step catalysed by isopenicillin N synthase (IPNS). This step is common to both penicillin and cephalosporin biosynthesis.
- In some organisms (e.g. Penicillium chrysogenum and Aspergillus nidulans) isopenicillin N is converted by exchange of its ½-δ-α-aminoadipoyl side chain to penicillins with other side chains, which are normally more hydrophobic than the side chain of isopenicillin N. This conversion is catalysed by an amidohydrolase/ acyltransferase enzyme. Examples of penicillins produced by this biosynthetic process include penicillin G (which has a phenylacetyl side chain) and penicillin V (which has a phenoxyacetyl side chain). These hydrophobic penicillins may be commercially produced via fermentation under the appropriate conditions.
 - 3. In other organisms (e.g. *Streptomyces clavuligerus* and *Cephalosporium acremonium*) isopenicillin N is epimerised to penicillin N.

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- 4. In some organisms (e.g. S. clavuligerus and C. acremonium) penicillin N is converted to DAOC. This reaction is catalysed by deacetoxycephalosporin C synthase (DAOCS) in some organisms (e.g. Streptomyces clavuligerus) and by deacetoxy/deacetylcephalosporin C synthase (DAOC/DACS) in others (e.g. C. acremonium).
- 5. In some organisms (e.g. *S. clavuligerus* and *C. acremonium*) DAOC is converted to deacetylcephalosporin C (DAC). This reaction is catalysed by deacetylcephalosporin C synthase (DACS) in some organisms (e.g. *S. clavuligerus*) and by deacetoxy/deacetylcephalosporin C synthase (DAOC/DACS) in others (e.g. *C. acremonium*).

Further biosynthetic steps to give other cephalosporin derivatives may also occur, e.g. in *C. acremonium* DAC may be converted to cephalosporin C and in *Streptomyces spp*. DAC may be converted to cephamycin C. The genes encoding for each of the enzymes catalysing steps 1-6 above have been identified and sequenced.

Fermented penicillins, cephalosporins and their biosynthetic intermediates are useful as antibiotics or as intermediates in the production of antibiotics. Penicillins with hydrophobic side chains may be used for the preparation of cephalosporins or intermediates used in the preparation of cephalosporins, e.g. penicillins (including penicillin G and penicillin V) may be used to prepare C-3 exomethylene cephams which may be used as intermediates in the preparation of the commercial antibiotics, e.g. Cefachlor.

The enzymes IPNS, DAOCS, DACS and DAOC/DACS are members of an extended family of Fe(II) utilising oxidase and oxygenase enzymes. Most of this family (including DAOCS, DACS and DAOC/DACS) utilise a 2-oxo acid (normally 2-oxoglutarate) as a cosubstrate in addition to dioxygen and the 'prime' substrate (e.g. penicillin N in the case of DAOCS). Since IPNS, does not use 2-oxoglutarate, it has a substantially different mechanism to the 2-oxoglutarate dependent oxygenases, and this gives

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rise to a significantly different active site.

The Invention

This invention is based on the determination of the three dimensional crystal structure of DAOCS and the information and developments which come from it. The X-ray co-ordinates provide very detailed 3-dimensional information on the relationships between amino acid residues in the structure of DAOCS and on the binding modes of the Fe-cofactor and the substrates to DAOCS. The structure allows the modification of DAOCS and related enzymes of penicillin and cephalosporin biosynthesis (including DACS and DAOC/DACS) in order to alter their substrate and product selectivities. Since the DAOCS structures are the first from the family of 2-oxoglutarate dependent dioxygenases they also allow for the design of new inhibitors of this family of enzymes. Previously partial overviews of the structures of IPNS complexed to manganese and IPNS complexed to iron and ACV were reported (Roach et al., Nature, 1995, 375, 700-704; Roach et al., Nature, 1997, 387, 827). The structures, as defined by their X-ray co-ordinates, of IPNS complexed to manganese and in complexes with iron, ACV and/or substrate

Procedures have been developed for the production of 7-aminodeacetoxycephaosporin C (7-ADCA) in which recombinant *P. chrysogenum* strains into which the DAOCS gene has been introduced are used for the production of cephalosporins. In particular if adipic acid is added to these recombinant strains adipoyl-6-APA is produced, which is converted by DAOCS into adipoyl-7-ADCA from which the adipoyl side chain can be removed (EPA-A-0532341, Shibata *et al.*, Bioorg. Med. Chem. Letts, 1996, 6, 1579-1584).

analogues have been reported in Baldwin, Hajdu, Roach, Hensgens,

Clifton, GB 9621486.1- (Oxygenase Enzymes and Method).

The IPNS gene sequence (and therefore the amino acid

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sequence) is related but significantly different to those of DAOCS, DACS, DAOC/DACS. It is likely that gross elements of the fold (i.e. significant elements within the 3-dimensional structure) of these enzymes will be conserved but that the active site architecture will be very significantly different. Structural elements conserved are likely to include the beta-barrel 'jelly roll' core and certain alpha-helices (including alpha helix-10, as defined in Roach et al., Nature, 1995, 375, 700-704). The degree of similarity is insufficient to define the precise structure of DAOCS, DACS, or DAOC/DACS from the IPNS structures. To date no models of DAOCS, DACS, or DAOC/DACS based on the IPNS structure have been reported. Nor have any detailed studies on substrate binding of these enzymes been reported. One report (WO 97/20053) claims the use of products resulting from modification of certain residues in DAOCS for the improved conversion of penicillin G to phenyl acetyl (G)-7-aminocephalosporanic acid.

The three-dimensional structure of DAOCS is defined by the X-ray co-ordinates set out below (Structure A).

Also set out below is a high resolution crystal structure of a complex of prokaryotic DAOCS from *S. clavuligerus* with Fe(II) and 2-oxoglutarate (Structure B).

In part the present invention relates to the use of the structures of DAOCS in order to make modifications to it or DACS or DAOC/DACS in order that the modified enzymes catalyse the conversion of unnatural penicillins (e.g. penicillin G and penicillin V) to cephalosporins more efficiently than the wild-type enzyme. Further aspects of the invention relate to the use of the DAOCS structure in order to produce unnatural products in micro-organisms. Such products include exomethylene cephalosporins, with or without alpha-aminoadipoyl or hydrophobic side chain (e.g. phenylacetyl or phenoxyacetyl). Thus one aspect of this invention refers to the use of the structure of DAOCS for modifying DAOCS

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(or the closely related enzymes DACS or DAOC/DACS) in order to:

- (i) permit the enzyme to accept (or accept more efficiently) unnatural penicillin substrates for the preparation of new or commercially valuable antibacterial materials.
- (ii) enable the modified enzyme to produce unnatural (e.g. exomethylene cephams) or optimise the production of minor products (e.g. $3-\beta$ -hydroxycephams) for use as antibacterials or as intermediates in the preparation of antibacterials or commercially valuable compounds.

In another aspect this invention provides modified enzymes that result from application of the aforementioned techniques. These are enzymes having significant (as defined below) sequence and thus structural similarity with DAOCS. Thus, structures of these enzymes may be predicted on the basis of the DAOCS structures. Preferably there will be sequence similarity/identity between most of the modified enzyme and a major part of DAOCS. Previous sequence comparisons (Roach et al., Nature, 1995, 375, 700), using pairwise comparisons of the sequences followed by single linkage cluster analysis show that IPNS, DAOCS, DACS and DAOC/DACS cluster with standard deviations scores of >5.0 (Barton and Sternberg, J. Mol. Biol., 1987, 198, 327). Scores over 5.0 and preferably over 6.0 indicate that the sequence alignments will be correct within all or most of the protein secondary structural elements (Barton, Methods in Enzymol., 1990, 183, 403); thus they have significantly similar sequences and hence structures. Note there are other criteria which may be used to ascertain significant sequence similarity for example % identity or % similarity of amino acids possessing side chains with similar physicochemical properties (Barton and Sternberg, J. Mol. Biol., 1987, 198, 327). Thus, on the basis of sequence comparisons it is possible to predict the structure of one enzyme (e.g. DACS or DAOC/DACS) from another closely related enzyme (e.g. DAOCS). Further, it is recognised that although two enzymes may have structures in which secondary structural elements are

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largely or wholly conserved, differences in the structures of the two enzymes may result from the side chains of the amino acids forming the secondary structural elements. The effect of these differences, which alter the substrate/product selectivities of the compared enzymes, is predictable once the three-dimensional structure of one of the enzymes is known.

In another aspect the invention provides an enzyme having significant (as herein defined) sequence similarity to DAOCS wherein the side chain binding site of penicillin N or DAOC is modified and at at least one of the following sites at least one amino acid residue is changed to another amino acid residue or is deleted: Thr72, Arg74, Arg75, Glu156, Leu158, Arg160, Arg162, Leu186, Ser187, Phe225, Phe264, Arg266, Asp301, Tyr302, Val303, Asn304; and/or at least one additional amino acid residue is inserted within the region 300-311; provided that other residues interacting with the above may be changed in order to accommodate the change in one of the above.

Modifications of this kind will permit the expansion of penicillin V or penicillin G to the corresponding cephalosporins. To achieve this it is desirable to increase the kcat/Km for the mutant as compared to the wild type DAOCS. Kinetic results indicate that apparent kcat values for penicillin N and penicillin G are similar but that Km is much higher for penicillin G. Thus based on these analysis, a decrease in the binding constant of DAOCS for penicillin G should make it possible to increase kcat/Km for penicillin G.

The side chain binding pocket of DAOCS is made of residues from different parts of the peptide chain, so it is likely that more than one residue will have to be altered to make a better penicillin G/V expander. Nevertheless some residues are more important than others. Examination of the interactions between the last few C-terminal residues (Thr-308 to Ala-311) of one DAOCS molecule and the active site of another in the crystal structure, suggests a binding mode for the penicillin nucleus which

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is shown in Figure 2 of the accompanying drawings. The penam C-3 carboxylate group probably occupies an analogous position to that of Ala-311 from a symmetry related molecule in the active site, forming electrostatic interactions with Arg-162 and Arg-160. The side chain of Arg-160 may also form a hydrogen bonding interaction with the β -lactam carbonyl.

It needs to be borne in mind that protein specificity is generally controlled by more than one amino acid. To alter the specificity of a protein in a major way is likely to require more than one of the mutational changes suggested below, although each of the mutations will contribute. With this in mind, preferred residues to modify for the expansion of a penicillin are as follows:

- a) Arg-266. This residue binds with the α -aminoadipate side chain of the natural substrate and should be changed to a residue of more hydrophobic character, e.g. Phe, Ala, Val, Leu, Ile.
- b) Thr-72. This should be changed to a hydrophobic residue e.g. Val, Leu, Ile, Phe, Ala, to help bind the hydrophobic side chain of penicillin G. It should be effective in combination with other mutants.
- c) Arg-74 may be usefully changed to a neutral or hydrophobic residue (Phe, Tyr, Val, Leu, Ile, Ala). Modification of Arg-75 may be necessary in addition because it forms a hydrogen-bonding network with Arg-74.
- d) Glu-156. This residue binds with the α -aminoadipate side chain. It should be changed to one of Ala, Val, Leu, Ile, Phe, Tyr, Trp, Asn, Gln, Ser.
- e) The side chains of Leu-158, Asn-301 and Tyr-302 form part of the binding pocket for the penicillin side chain and can be usefully modified to more hydrophobic character.
 - f) Asn-304. This residue binds the amide linking the side chain to the penam nucleus. Modification is effected to expand penicillins with shortened or no side chains (e.g. to Asp or Glu for 6-Apa).

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Note that other changes may be used to construct part or all of a side chain binding pocket via hydrogen bonding or other interactions.

The insertion or deletion of residues into the DAOCS sequence may also be of use in constructing a hydrophobic binding pocket for the penicillin side chain. Insertion of hydrophobic residues into the C-terminal region (residue 300-311 and in particular 301-303) may assist in the construction of a hydrophobic binding pocket for penicillin side chains.

In another aspect the invention provides an enzyme having significant (as herein defined) sequence similarity to DAOCS wherein the penicillin/cephalosporin binding site of penicillin N or DAOC is modified and at at least one of the following amino acid residues is changed or deleted: Ile88, Arg160, Arg162, Phe164, Met180, Thr190, Ile192, Phe225, Pro241, Val245, Val262, Phe264, Asn304, Ile305, Arg306, Arg307; and/or at least one additional amino acid residue is inserted within the region 300-311; provided that other residues interacting with the above may be changed in order to accommodate the change in one of the above.

Further discussion of this aspect may be found in Nature Volume 394, pages 805-809 published on 20 August 1998 and incorporated by reference herein.

Another aspect of the invention refers to the use of the structure of DAOCS in order to modify its active site (or that of a structurally related 2-oxoglutarate dependent dioxygenase) in order that the modified enzyme accepts non beta lactam substrates in order to produce oxidised compounds of value. Oxidised amino acids (e.g. 4-hydroxyprolines, hydroxylysines, hydroxyaspartic acids and others) are useful as synthetic intermediates in the production of valuable materials. Using the structure of DAOCS specific residues can be targeted for modification in order that the modified enzyme can be used to produce oxidised amino acids or peptides. The process may include modification of the following residues:

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Arg74, Glu156, Leu158, Arg160, Arg162, Leu186, Ser187, Phe225, Phe264, Arg266, Asp301, Tyr302, Val303, Asn304, Ile88, Arg162, Phe164, Met180, Thr190, Ile192, Pro241, Val245, Val262, Ile305, Arg306, Arg307.

Another aspect of the invention refers to the use of the DAOCS structure for the design of selective inhibitors of 2-oxoglutarate dependent dioxygenases. The 2-oxoglutarate dependent dioxygenase prolyl 4-hydroxylase has been the target of inhibition in order to provide a therapeutic treatment for fibrotic diseases (e.g. liver cirrhosis, arthritis). However, no inhibitors are in clinical use, probably because it is difficult to achieve selective inhibition of the target enzyme for inhibition over other enzymes (including 2-oxoglutarate dependent enzymes). The structure of DAOCS provides a template for the design of inhibitors of 2-oxoglutarate dependent dioxygenases.

Set out below are two high resolution crystal structures for DAOCS from *S. clavuligerus*: the structure of the iron-free apoenzyme (Structure A) and the structure of the complex with Fe(II) and 2-oxoglutarate (Structure B). The results imply a mechanism by which the enzyme-Fe(II) complex reacts with 2-oxoglutarate and dioxygen to give the reactive ferryl species, a process common to many non-haem oxygenases. Other notable 2-oxoacid-dependent ferrous enzymes are prolyl hydroxylase, involved in collagen biosynthesis, gibberellin 3β -hydroxylase, a mutation of which influences stem length in plants, and clavaminic acid synthase, involved in the biosynthesis of the β -lactamase inhibitor, clavulanic acid. Within the family of 2-oxoacid-dependent enzymes, DAOCS belongs to a sub-family, the members of which show sequence similarity with IPNS and 1-aminocyclopropane-1-carboxylate oxidase (the ethylene forming enzyme), enzymes that do not use a 2-oxoacid in catalysis.

The iron-free form of DAOCS crystallises in space group R3

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as a crystallographic trimer. The main chain of the protein folds into a conserved jelly roll core with flanking helices.

Co-ordinates and structure factors have been deposited with the Protein Data Bank (entries 1rxg, and r1rxgsf for the Fe(II)-2-oxoglutarate complex).

LEGENDS TO FIGURES.

Figure 1: the biosynthetic pathway to the penicillins and cephalosporins.

Figure 2 is a view of the active site of DAOCS showing 2-oxoglutarate binding to the iron and proposed penicillin N binding. Interactions with the side chains of certain amino acid residues are indicated by arrows.

Structure A is a three-dimensional structure of DAOCS.

Structure B is a high resolution crystal structure for prokaryotic DAOCS from *S. clavuligerus* as a complex with Fe(II) and 2-oxoglutarate.

The peptide sequence of DAOCS (with the numbering used herein) is set out below:

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		Met	Asp	Thr	Thr	Val	Pro	Thr	Phe	Ser	Leu	10
		Ala	Glu	Leu	Gln	Gln	Gly	Leu	His	Gln	Asp	20
		Glu	Phe	Arg	Arg	Cys	Leu	Arg	Asp	Lys	Gly	30
		Leu	Phe	Tyr	Leu	Thr	Asp	Cys	Gly	Leu	Thr	40
	5	qaA	Thr	Glu	Leu	Lys	Ser	Ala	Lys	Asp	Leu	50
		Val	Ile	Asp	Phe	Phe	Glu	His	Gly	Ser	Glu	60
		Ala	Glu	Lys	Arg	Ala	Val	Thr	Ser	Pro	Val	70
		Pro	Thr	Met	Arg	Arg	Gly	Phe	Thr	Gly	Leu	80
		Glu	Ser	Glu	Ser	Thr	Ala	Gln	Ile	Thr	Asn	90
Market III	10	Thr	Gly	Ser	Tyr	Ser	Asp	Tyr	Ser	Met	Cys	100
		Tyr	Ser	Met	Gly	Thr	Ala	Asp	Asn	Leu	Phe	110
or state of the control of the contr		Pro	Ser	Gly	Asp	Phe	Gly	Arg	Ile	Trp	Thr	120
		Gln	Tyr	Phe	qzA	Arg	Gln	Tyr	Thr	Ala	Ser	130
		Arg	Ala	Val	Ala	Arg	Glu	Val	Leu	Arg	Ala	140
# 4	15	Thr	Gly	Thr	Glu	Pro	Asp	Gly	Gly	Val	Glu	150
		Ala	Phe	Leu	Asp	Cys	Glu	Pro	Leu	Leu	Arg	160
		Phe	Arg	Tyr	Phe	Pro	Gln	Val	Pro	Glu	His	170
		Arg	Ser	Ala	Glu	Glu	Gln	Pro	Leu	Arg	Met	180
Andrews		Ala	Pro	His	Tyr	Asp	Leu	Ser	Met	Val	Thr	190
	20	Leu	Ile	Gln	Gln	Thr	Pro	Cys	Ala	Asn	Gly	200
		Phe	Val	Ser	Leu	Gln	Ala	Glu	Val	Gly	Gly	210
		Ala	Phe	Thr	Asp	Leu	Pro	Tyr	Arg	Pro	Asp	220
		Ala	Val	Leu	Val	Phe	Cys	Gly	Ala	Ile	Ala	230
		Thr	Leu	Val	Thr	Gly	Gly	Gln	Val	Lys	Ala	240
	25	Pro	Arg	His	His	Val	Ala	Ala	Pro	Arg	Arg	250
		Asp	Gln	Ile	Ala	Gly	Ser	Ser	Arg	Thr	Ser	260
		Ser	Val	Phe	Phe	Leu	Arg	Pro	Asn	Ala	Asp	270
		Phe	Thr	Phe	Ser	Val	Pro	Leu	Ala	Arg	Glu	280
		Cys	Gly	Phe	Asp	Val	Ser	Leu	Asp	Gly	Glu	290
	30	Thr	Ala	Thr	Phe	Gln	Asp	Trp	Ile	Gly	Gly	300
		Asn	Tyr	Val	Asn	Ile	Arg	Arg	Thr	Ser	Lys	310
		Ala										311

STRUCTURE A

CRYST1	106.400	106.40	71.10	0	90.00	90.00	120.00
SCALE1	0.009	9398	0.005426	0.0000	00	0.0000	00
SCALE2	0.000	0000	0.010852	0.0000	00	0.0000	00
SCALE3	0.000	0000	0.000000	0.0140	65	0.0000	00

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ATOM ANISOU ATOMOU ANISOU	22 22 23 23 24	OD1 OD2 OD2 N N CA C C O O CB CG CG SD CE	AMETT 1 BMETT 1 BMETT 1 BMETT 1 BMETT 1 BMETT 1 BMETT 1	8315 30.985 9037 30.472 4807 29.961 3925 29.77 28.67 27.626 27.564 6146 28.30 29.57 28.67 27.564 6146 28.30 30.592 467.993 28.67 29.97 28.67 29.97 28.67 29.97 29.97 28.67 29.97	-13- 10.641 2319 11.769 3006 12.900 3113 12.670 2381 11.328 3692 12.015 4873 11.232 7957 11.973 2111 14.105 3022 15.322 2803 15.268 1997 15.650 5248 16.528 3085 17.862 2611 17.937 504 817.862 2611 17.937 504 811.857 2613 11.840 5740 11.495 3819 12.079	59.03 59.06 59.06 59.06 59.06 59.06 59.08 61.07 58.02 57.90 56.67 59.06 53.15 59.06 53.15 59.06 53.15 59.06 59	-614 0.542 -78642 -0.542 0.5442 0.542 0.542 0.542 0.542 0.542 0.542 0.542 0.542 0.5442 0.5	39.90 -1026 - 296 28.97 -2189 - 119 28.12 -1097 7 4 34.85 1 - 373 38.19 912 - 1765 47.19 1050 - 1326 27.10 -1467 - 9 30.20 -782 - 383 34.22 -964 - 525 33.34 -1457 8 7 7 44.76 -1582 1631 25.98 -1794 5 8 2 38.05 -608 - 1114 42.35 0 1991 28.59 -1022 - 253 29.49 1580 4 7 7 40.62 210 103 38.21 -909 - 915 44.81 -656 - 12 33.14 -122 8 1 8 40.28 -751 5 3 34.23 -215 2 0
ANISOU ATOM ANISOU ATOM ANISOU ATOM	19 20 20 21 21 22	C O O CB CB CG	BMET 1 BMET 1 BMET 1 BMET 1 BMET 1 BMET 1	5082 30.075 8292 31.131 4866 29.625	14.113 3637 14.599 3208 11.857 2613 11.840	57.894 5797 57.110 5525 56.829 5114 56.968	0.458 282 0.458 2071 0.458 2013 0.458	38.21 -909 - 915 44.81 -656 - 12 33.14 -122 818 40.28
ATOM ANISOU	23 23 24 24 25 25 26 26	SD SD	BMET 1 BMET 1	28.761 5619	11.495 3819	55.422	0.458 2050 0.458 1149 0.732 -1323 0.732	34.23 -21520 54.24 4083-2463 37.72 -1208-1385
ATOM ANISOU ATOM ANISOU ATOM ANISOU ATOM	27 27 28	C C O O C C C C	BASP 2 BASP 2 BASP 2 BASP 2 BASP 2 BASP 2 BASP 2 BASP 2	28.536 4876 28.181 4375 30.195 6632 29.562 3243 28.866	14.886 1624 14.602 3689 16.696 3351 17.730 3791 17.247	59.567 4771 58.414 5100 59.181 4222 60.104 4510 61.030	0.732 27 -19 0.732 65 -10 0.732 -1850 0.732 -500	29.66 561 1218 34.65 485 247 37.39 869 -1518 30.38 -606 -1191

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ANISOU 31 ATOM 32	OD1 BASP 2 OD2 BASP 2	6276	4203	8095	-1203 3147 -1901	
ANISOU 32	OD2 BASP 2	29.760 2852	18.945 3708	59.875	0.732 34.85 -491 444 -1450	
ATOM 33	N THR 3	27.717	14.789		1.000 35.58	
ANISOU 33 ATOM 34	N THR 3 CA THR 3	4586	4123	4811	601 -1628 1516	5
ANISOU 34	CA THR 3 CA THR 3	26.303 4650	14.433 4555	60.495 6175	1.000 40.48 371 -911 - 385	
ATOM 35	C THR 3	25.382	15.647		371 -911 - 385 1.000 39.82	
ANISOU 35	C THR 3	4376	4155	6598	320 -3864 -586	5
ATOM 36 ANISOU 36	O THR 3 O THR 3	24.150 4668	15.556 3107	60.751 4972	1.000 33.55 357 -2748 -588	_
ATOM 37	CB THR 3	25.905	13.450		357 -2748 -588 1.000 39.95	3
ANISOU 37	CB THR 3	3787	4004	7387	160 -1209 6 2	
ATOM 38 ANISOU 38	OG1 THR 3 OG1 THR 3	26.591 10134	13.851 5882	62.817 7476	1.000 61.83 -4164 -3020 205:	1
ATOM 39	CG2 THR 3	26.399	12.052		-4164 -3020 205: 1.000 59.32	T
ANISOU 39	CG2 THR 3	4613	3971	13955	1114 -3135 -198	3
ATOM 40 ANISOU 40	N THR 4 N THR 4	26.036 4306	16.780 4611		1.000 32.55 377 -2166 -21	_
ATOM 41	CA THR 4	25.439	18.092	3450 60.393	377 -2166 -21' 1.000 31.22	/
ANISOU 41	CA THR 4	4275	4229	3358	-81 -1179 9 5	
ATOM 42 ANISOU 42	C THR 4 C THR 4	24.672 4876	18.272 3341	59.090 3207	1.000 30.06 773 -1156 -20	s
ATOM 43	O THR 4	25.195	17.935		773 -1156 -204 1.000 31.64	4
ANISOU 43	O THR 4	4877	3780	3363	1935 -1255 - 52	
ATOM 44 ANISOU 44	CB THR 4 CB THR 4		19.208 4762	60.407 5194	1.000 32.31	
ATOM 45	OG1 THR 4	27.324	19.091		475 -547 5 9 3 1.000 3 2 . 3 6	
ANISOU 45	OG1 THR 4	3705	3955	4635	-79 -797 -389	
ATOM 46 ANISOU 46	CG2 THR 4 CG2 THR 4	25.852 3728	20.582 4174	60.458 2443	1.000 27.22	
ATOM 47	N VAL 5	23.464	18.796		71 304 - 151 1.000 21.69	
ANISOU 47	N VAL 5	4041	1985	2215	-543 -657 1 5 8	
ATOM 48 ANISOU 48	CA VAL 5 CA VAL 5	22.690 3 6 75	19.140 1964		1.000 20.42	
ATOM 49	C VAL 5	23.199	20.489	2120 57.499	-622 -517 1 0 3 1.000 17.01	
ANISOU 49	C VAL 5	2263	1803	2396	-279 -622 8 9	
ATOM 50 ANISOU 50	O VAL 5 O VAL 5	23.156 3662	21.449		1.000 21.10	
ATOM 51	CB VAL 5	21.204	1885 19.216	2472 58.402	-389 -656 1 6 1.000 24.22	
ANISOU 51	CB VAL 5	3551	2155	3495	-1045 -396 783	
ATOM 52 ANISOU 52	CG1 VAL 5	20.434 3202	19.700	57.166	1.000 20.14	
ATOM 53	CG2 VAL 5	20.701	1779 17.867	2672 58 860	-453 10 -226 1.000 28.58	
ANISOU 53	CG2 VAL 5	5258	2086	3516	-1226 431 510	
ATOM 54 ANISOU 54	N PRO 6 N PRO 6	23.750 2378	20.542		1.000 16.95	
ATOM 55	CA PRO 6	24.354	1629 21.793	2434 55.857	29 -594 3 0 1 1.000 16.90	
ANISOU 55	CA PRO 6	1645	1775	3000	6 -445 303	
ATOM 56 ANISOU 56	C PRO 6 C PRO 6	23.298 1477	22.800		1.000 15.61	
ATOM 57	O PRO 6	22.133	1766 22.432	2687 55.201	-192 -437 5 4 5 1.000 15.75	
ANISOU 57	O PRO 6	1578	1761	2647	-260 -579 5 5	
ATOM 58 ANISOU 58	CB PRO 6 CB PRO 6	25.216 2320	21.375 1752		1.000 19.85	
ATOM 59	CG PRO 6	24.632	20.095	3468 54.187	50 70 1 8 2 1.000 2 4 . 7 6	
ANISOU 59	CG PRO 6	3550	2953	2904	-1186 300 - 286	
ATOM 60 ANISOU 60	CD PRO 6 CD PRO 6		19.428	55.357	1.000 17.91	
ATOM 61	N THR 7		1962 24.031	2882 55.156	-168 -138 - 44 1.000 14.38	
ANISOU 61	N THR 7		1567	2378	-158 -616 1 0 0	

- 15 -

CA THR 7 22.907 25.103 54.610 1.000 14.09 ATOM 62 ANISOU 62 CA THR 7 1625 1554 2174 -255 -581 2 2 8 7 MOTA 63 С THR 23.605 25.684 53.374 1.000 14.74 C 7 ANISOU 63 THR 1683 1849 2067 -193 -468 1 2 1 64 0 THR 7 25.894 53.423 1.000 15.95 MOTA 24.828 7 ANISOU 64 0 THR 1752 2137 2171 -378 -457 1 8 5 THR 7 22.795 ATOM 65 СВ 26.248 55.637 1.000 15.25 CB THR 7 ANISOU 65 1548 56 -124 5 2 1846 2401 OG1 THR 7 22.208 25.717 56.829 1.000 16.91 ATOM 66 2149 OG1 THR 7 -402 -183 4 7 ANISOU 66 1818 2458 CG2 THR 7 67 21.952 27.387 55.040 1.000 16.09 MOTA 7 ANISOU 67 CG2 THR 1651 1613 2848 -138 -263 - 25 MOTA 68 N PHE 8 22.830 25.892 52.325 1.000 15.06 ANISOU 68 1966 2137 Ν PHE 8 1618 -411 -558 2 3 0 MOTA 69 CA PHE 8 23.317 26.545 51.136 1.000 14.76 ANISOU 69 CA PHE 8 1857 1558 2192 -213 -411 2 8 1 70 С PHE 22.421 27.728 ATOM 8 50.810 1.000 14.94 ANISOU 70 С PHE 1907 8 1421 2347 -275 -357 1 8 1 PHE 71 0 8 21.198 27.678 50.995 1.000 16.40 ATOM ANISOU 71 0 PHE 8 1782 1642 2808 -197 -550 3 4 CB PHE CB PHE 25.562 MOTA 72 8 23.242 49.948 1.000 16.49 ANISOU 72 8 2123 1854 2287 49 -371 - 1 PHE 50.027 1.000 14.92 ATOM 73 CG 8 24.225 24.432 ANISOU 73 CG PHE 8 1710 1824 2135 -197 -365 1 6 3 CD1 PHE 50.600 1.000 16.78 23.822 ATOM 74 8 23.227 ANISOU 74 CD1 PHE 1726 2842 -300 -358 1 8 4 8 1808 75 CD2 PHE 25.539 24.558 49.602 1.000 16.67 ATOM 8 ANISOU 75 CD2 PHE 8 1705 2130 2500 -310 -361 3 2 1 76 CE1 PHE 50.742 1.000 16.74 ATOM 8 24.702 22.183 ANISOU 76 CE1 PHE 8 2035 1966 2359 -4 -99 2 9 5 ATOM 77 CE2 PHE 8 26.420 23.525 49.773 1.000 19.18 ANISOU 77 CE2 PHE 8 1398 2153 3736 **-4**08 **-631 1 8 7** CZ PHE 50.351 1.000 17.90 MOTA 78 8 26.026 22.336 ANISOU 78 CZ PHE 8 1849 -119 -376 2 0 2003 2948 MOTA 79 N SER 9 23.023 28.776 50.314 1.000 14.82 ANISOU 79 SER 9 2134 1488 2008 -351 -528 3 1 0 N 49.715 1.000 15.12 ATOM 80 CA SER 9 22.338 29.902 ANISOU 80 9 CA SER 2037 1259 2449 -357 -571 1 3 4 48.270 1.000 16.19 ATOM 81 SER 9 21.977 С 29.607 2224 ANISOU 81 С SER 9 2138 1791 -374 -535 5 4 7 MOTA 82 0 SER 9 22.877 29.312 47.473 1.000 17.04 ANISOU 82 9 0 SER 2191 1892 2393 -423 -544 2 3 2 MOTA 83 CB SER 9 23.306 31.113 49.696 1.000 18.74 ANISOU 83 СВ -1012 -478 7 1 7 SER 9 2891 1712 2519 ATOM 84 OG SER 9 22.738 32.131 48.853 1.000 20.82 ANISOU 84 OG SER 9 1569 3477 -662 -854 6 0 7 2866 ATOM 85 LEU 10 20.697 29.674 47.924 1.000 16.46 N -228 -740 - 48 ANISOU 85 N LEU 10 2215 1495 2542 MOTA 86 CA LEU 10 20.345 29.401 46.529 1.000 17.55 ANISOU 86 CALEU 10 2263 1856 2551 -582 -694 3 6 ATOM 87 C LEU 10 21.079 30.373 45.591 1.000 18.84 С ANISOU 87 LEU 10 2506 1870 -596 -830 3 5 7 2784 8.8 LEU ATOM 0 10 21.573 30.025 44.520 1.000 20.19 ANISOU 88 Ο LEU 10 2705 2704 -524 -663 5 0 8 2263 MOTA 89 CB LEU 10 18.844 29.559 46.327 1.000 18.87 ANISOU 89 CB LEU 10 2302 2516 2354 -288 -715 2 8 0 CG LEU 29.333 MOTA 90 10 18.355 44.895 1.000 18.28 ANISOU 90 10 2182 2172 2591 -668 -677 - 301 27.955 44.397 1.000 22.45 ATOM 91 CD1 LEU 10 18.708 3089 -308 -537 1 7 ANISOU 91 CD1 LEU 10 3418 2024

16.852 29.603 44.869 1.000 21.93

10

CD2 LEU

92

ATOM

- 16 -

ANISOU 92 CD2 LEU 10 2250 2658 3424 -504 -1139 7 5 ATOM 93 N ALA 11 21.154 31.638 46.037 1.000 20.05 N ALA 11 2862 ANISOU 93 1780 2977 -595 -1279 472 MOTA 94 CA ALA 11 45.202 1.000 24.24 21.810 32.647 ANISOU 94 CA ALA 11 3160 1670 4380 -455 -979 8 9 1 C 95 ATOM ALA 11 23.285 32.309 44.946 1.000 21.06 ANISOU 95 ALA11 3128 1937 2937 -644 -1016 431 ATOM 96 0 11 23.819 32.447 ALA 43.829 1.000 26.29 ANISOU 96 0 ALA 11 3569 3261 3158 -1628 -923 1137 CB ALA 97 ATOM 11 21.752 33.989 45.953 1.000 24.29 ANISOU 97 11 3740 1692 3797 -461 -216 9 9 6 ATOM 98 23.953 31.844 46.005 1.000 20.65 N GLU 12 ANISOU 98 N GLU 12 2829 1975 3044 -828 -930 674 ATOM 99 CA GLU 12 25.354 31.463 45.862 1.000 21.19 ANISOU 99 CA GLU 12 3036 2400 2615 -506 -715 5 9 8 ATOM 100 C 25.483 30.277 44.920 1.000 21.56 GLU 12 ANISOU 100 C GLU 12 3894 2179 2117 -702 -206 9 8 8 101 0 MOTA 12 GLU 26.375 30.215 44.069 1.000 21.98 ANISOU 101 O GLU 12 3463 2917 1971 -1144 -488 6 1 8 102 CB GLU ATOM 12 26.032 31.170 47.204 1.000 20.27 ANISOU 102 CB GLU 12 2874 2192 2636 -221 -624 5 0 1 ATOM 103 CG GLU 12 26.156 32.451 48.032 1.000 20.54 ANISOU 103 CG GLU 12 2889 2316 -344 -516 4 0 6 2598 ATOM 104 CD GLU 12 26.787 32.279 49.389 1.000 21.86 ANISOU 104 CD GLU 12 3146 2542 ATOM 105 OE1 GLU 12 27.068 31.149 49.803 1.000 24.98

ANISOU 105 OE1 GLU 12 3642 2681 3169 -1348 -1088

ATOM 106 OE2 GLU 12 26.819 33.305 50.092 1.000 33.52

ANISOU 106 OE2 GLU 12 5881 2966 3888 -1119 -2251

ATOM 107 N LEU 13 24.600 29.295 45.060 1.000 18.91

ANISOU 107 N LEU 13 2567 2345 2275 -351 -390 3

ATOM 108 CA LEU 13 24.645 28.117 44.174 1.000 18.61 2619 -1297 -612 7 9 9 -1348 -1088 1134 -1119 -2251 4 6 ANISOU 109 C LEU ANISOU 2275 -351 -390 3 8 2 13 24.645 28.117 44.174 1.000 18.61 13 2575 2347 2149 -209 270 406 13 24.432 28.566 42.738 1.000 21.40 13 3827 3216 1981 -823 -117 1 13 23.541 27.137 44.562 1.000 18.97 13 2982 2243 1984 -462 1165 13 3558 2367 -709 -41 526 -823 -117 1 9 0 111 CB LEU MOTA ANISOU 111 CB LEU -462 -145 4 4 0 112 CG LEU MOTA ANISOU 112 CG LEU 2322 13 2313 2422 -467 -362 7 4 5 CD1 LEU ATOM 113 22.526 25.480 46.070 1.000 20.74 13 ANISOU 113 CD1 LEU 13 2769 2266 2845 -789 -142 5 9 4 114 CD2 LEU ATOM 13 25.023 25.473 45.858 1.000 19.80 ANISOU 114 CD2 LEU 13 2709 2229 2585 -244 -509 - 107 115 N GLN 14 23.544 29.508 ATOM 42.478 1.000 22.03 ANISOU 115 N GLN 14 3596 2139 2635 -960 -903 3 7 9 ATOM 116 CA GLN 14 23.284 29.978 41.104 1.000 23.79 ANISOU 116 CA GLN 14 3010 3335 2694 -992 -816 648 117 C ATOM GLN 14 24.481 30.712 40.509 1.000 25.44 ANISOU 117 C GLN 143360 3427 2881 -1070 -382 4 8 7 118 0 MOTA 14 24.655 30.829 GLN 39.288 1.000 30.04 ANISOU 118 O GLN 14 3836 4657 2922 -1208 -427 8 9 8 ATOM 119 CB GLN ANISOU 119 CB GLN ATOM 120 CG GLN ANISOU 120 CG GLN 14 22.064 30.906 41.131 1.000 26.28 14 3133 3630 3222 -760 -863 9 3 8 14 20.772 30.111 41.355 1.000 23.26 14 3106 2319 3413 -299 -577 5 1 4 MOTA 121 CD GLN 14 19.586 31.020 41.631 1.000 23.69 ANISOU 121 CD GLN 14 3384 2462 3155 -317 -393 - 196 ATOM 122 14 19.734 32.104 42.160 1.000 28.34 OE1 GLN ANISOU 122 OE1 GLN 14 4973 2619 3175 -183 -732 -408

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123 NE2 GLN 14 18.398 30.513 41.349 1.000 23.60
 ATOM 123 NE2 GLN 14 18.398 30.513 41.349 1.000 23.60 ANISOU 123 NE2 GLN 14 3058 2969 2941 -383 54 24 9 ATOM 124 N GLN 15 25.309 31.243 41.395 1.000 25.00 ANISOU 124 N GLN 15 3078 3281 3140 -1159 -394 5 ATOM 125 CA GLN 15 26.530 31.936 40.945 1.000 24.05 ANISOU 125 CA GLN 15 2947 3560 2631 -866 -98 6 ATOM 126 C GLN 15 27.650 30.920 40.707 1.000 26.06 ANISOU 126 C GLN 15 3810 3951 2139 -345 406 6 ATOM 127 O GLN 15 28.756 31.284 40.302 1.000 35.85 ANISOU 127 O GLN 15 4294 4851 4476 102 1871 17 ATOM 128 CB GLN 15 3055 3037 3748 -1092 -109 3 ATOM 129 CG GLN 15 26.103 34.092 42.219 1.000 31.24 ANISOU 129 CG GLN 15 4562 2577 4731 -806 962 16
  ATOM
                                                                               2941 -383 54 2 4 5
                                                                              3140 -1159 -394 5 7 5
                                                                3560 2631 -866 -98 655
                                                                3951 2139 -345 406 668
                                                                4851 4476 102 1871 1192
                                          15 3055 3037 3748 -1092 -109 3 6 4
15 26.103 34.092 42.219 1.000 31.24
  ANISOU 129 CG GLN
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15 26.503 35.022 43.348 1.000 59.75
  ATOM 130 CD GLN
  ANISOU 130 CD GLN
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27.634 35.031 43.840 1.000 81.81
            131 OE1 GLN 15
  ATOM
  ANISOU 131 OE1 GLN 15
              131 OE1 GLN 15 15059 3931 12094 -944 -6272 -1803 132 NE2 GLN 15 25.539 35.841 43.767 1.000 91.46
                                                15059
  ATOM
 ANISOU 132 NE2 GLN 15 14070 4846 15833 -923 3672 -4850 ATOM 133 N GLY 16 27.379 29.643 40.969 1.000 29.90 ANISOU 133 N GLY 16 4634 3820 2907 -239 22 787
ANISOU 133 N GLY 16 4634 3820 2907 -239 22 78 7 ATOM 134 CA GLY 16 28.410 28.649 40.699 1.000 28.76 ANISOU 134 CA GLY 16 29.339 28.473 41.878 1.000 27.60 ANISOU 135 C GLY 16 29.339 28.473 41.878 1.000 27.60 ANISOU 136 O GLY 16 30.398 27.867 41.725 1.000 31.47 ANISOU 136 O GLY 16 3386 4758 3814 -899 1243 10 ATOM 137 N LEU 17 28.960 28.898 43.083 1.000 26.01 ANISOU 137 N LEU 17 3295 3636 2950 -721 162 74 ATOM 138 CA LEU 17 29.776 28.666 44.257 1.000 23.96 ANISOU 138 CA LEU 17 2700 3032 3372 -601 100 6 ANISOU 138 CA LEU 17 2700 3032 3372 -601 100 6 ANISOU 138 CA LEU 17 2700 3032 3372 -601 100 6 ANISOU 139 C LEU 17 29.462 27.338 44.932 1.000 20.31 ANISOU 139 C LEU 17 2222 2763 2733 -252 611 26 ATOM 140 O LEU 17 28.389 26.780 44.789 1.000 20.31 ANISOU 140 O LEU 17 2347 3134 3308 -443 263 89 ANISOU 141 CB LEU 17 29.645 29.806 45.286 1.000 25.94 ANISOU 141 CB LEU 17 28.86 2933 4035 -1318 -405 29 ATOM 142 CG LEU 17 29.962 31.209 44.716 1.000 31.57 ANISOU 142 CG LEU 17 29.9550 32.358 45.615 1.000 32.04
                                                                              2833 -709 461 250
                                                                              2891 -616 914 1485
                                                                              3814 -899 1243 1023
                                                                                           -721 162 743
                                                                                            -601 100 673
                                                                                            -252 611 261
                                                                                            -443 263 859
                                                                                            -1318 -405 2 5 4
                                                                              5308 -523 1150 7 2 2
            143 CD1 LEU
                                        17 29.550 32.358 45.615 1.000 32.04
  ANISOU 143 CD1 LEU
                                        17 5221
                                                                2887
                                                                              4066
                                                                                           -1269 278 508
            144 CD2 LEU 17 31.458 31.278 44.416 1.000 38.11
  ATOM
  ANISOU 144 CD2 LEU 17 3828
                                                                5491
                                                                              5160 -2315 954 232
                                                                26.822 45.681 1.000 22.49
  ATOM
            145 N HIS 18 30.441
  ANISOU 145 N
                               HIS
                                         18 2600
                                                                3067
                                                                               2877
                                                                                           -662 42 4 4 9
            146 CA HIS
  ATOM
                                        18 30.289 25.644 46.537 1.000 21.54
 ANISOU 146 CA HIS
                                         18 2378
                                                                2809
                                                                               2996
                                                                                           -432 201 313
 ATOM 147 C HIS
ANISOU 147 C HIS
ATOM 148 O HIS
                                         18 29.908 24.376 45.790 1.000 22.76
                                         18 2256
                                                                3245
                                                                               3148 -1009 282 114
                                         18 29.147 23.565 46.331 1.000 22.60
 ANISOU 148 O HIS
ATOM 149 CB HIS
ANISOU 149 CB HIS
ATOM 150 CG HIS
ANISOU 150 CG HIS
                                          18 2008
                                                                3064
                                                                               3516
                                                                                           -629 -166 8 8 4
                                         18 29.224 25.872 47.618 1.000 22.81
                                         18 2514
                                                                2879
                                                                               3272 -526 450 421
                                         18 29.320 27.248 48.217 1.000 21.70
                                         18 2797
                                                                3038
                                                                               2411 -149 39 5 0 3
  ATOM
                       ND1 HIS
               151
                                         18 30.438
                                                              27.773 48.807 1.000 25.01
  ANISOU 151
                        ND1 HIS
                                          18 3714
                                                                               2284 -207 -629 1 4 9
                                                                3505
  MOTA
               152
                        CD2 HIS
                                          18 28.370 28.216 48.269 1.000 24.95

    18
    3244
    3278
    2957
    87 544 2 7 5

    18
    30.197
    28.982
    49.223
    1.000 29.26

  ANISOU 152
                        CD2 HIS
  ATOM 153
                       CE1 HIS
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ANISOU 153 ATOM 154 ANISOU 155 ANISOU 155 ANISOU 156 ANISOU 156 ATOM 157 ANISOU 157 ANISOU 157 ANISOU 158 ATOM 158 ANISOU 158 ATOM 159 ANISOU 159 ATOM 160 ANISOU 160 ATOM 161 ANISOU 161 ANISOU 161 ANISOU 162 ANISOU 163 ANISOU 163 ANISOU 163 ANISOU 163 ANISOU 165 ANISOU 165 ANISOU 166 ANISOU 166 ANISOU 166 ANISOU 166 ANISOU 166 ANISOU 167 ANISOU 167 ANISOU 167 ANISOU 168 ATOM 168 ATOM 168 ATOM 169 ANISOU 169 ANISOU 170 ANISOU 170 ANISOU 170 ANISOU 171 ANISOU 171 ANISOU 172 ANISOU 173 ANISOU 174 ANISOU 175 ANISOU 175 ANISOU 176 ANISOU 177	C GLU 21 O GLU 21 CB GLU 21 CB GLU 21 CG GLU 21 CG GLU 21 CD GLU 21 CD GLU 21 CD GLU 21	1386 2342 28.290 19.6 1671 2286 30.415 22.0 1646 2821 31.893 22.3 1682 3568 32.574 23.3 1330 4241 32.249 23.5	3118 71 48.919 2632 70 44.521 2822 13 43.730 3263 60 44.221 3095 01 44.259 3574 22 42.276 2947 33 41.523 3508 68 41.862 4521 72 44.631 3123 92 45.225 3235 42 46.546 2873 99 46.768 3848 68 45.521 4130 06 44.291 5705 14 43.153 4992 33 44.467 6277 53 47.404 3093 11 48.665 2838 48.402 3050 02 49.054 3057 58 49.563 3170 22 49.918 3912 80 49.081 5713 94 47.887	-388	. 5 7
ANISOU 175 ATOM 176 ANISOU 176 ATOM 177 ANISOU 177 ATOM 178	O GLU 21 CB GLU 21 CB GLU 21 CG GLU 21 CG GLU 21 CD GLU 21	1671 2286 30.415 22.0 1646 2821 31.893 22.3 1682 3568 32.574 23.3	3057 58 49.563 3170 22 49.918 3912 80 49.081	-419 -351 1 1 6 1.000 20.10 -514 -499 1 2 7 1.000 24.11 -766 -326 - 7 1 1 1.000 29.70	L
			5713 94 47.887 6677 07 49.678 6860 48 47.395 2680 61 47.071 2807 29 46.552	-752 -666 5 2 1 1.000 35.14 -1336 -1741 19 1.000 39.39 -2089 -1618 6 4 1.000 17.30	

- 19 -ATOM 184 0 PHE 22 25.867 18.574 46.995 1.000 15.87 ANISOU 184 0 PHE 22 1570 2118 2343 -249 -361 1 3 1 ATOM 185 CB PHE 22 26.305 21.840 46.149 1.000 18.00 ANISOU 185 СВ PHE 22 1747 2754 2337 70 -178 445 21.729 186 CG 22 MOTA PHE 24.802 45.930 1.000 16.38 ANISOU 186 CG PHE 22 1763 1748 2714 -90 -326 2 2 3 187 CD1 PHE 22 23.934 21.723 47.003 1.000 18.29 MOTA ANISOU 187 CD1 PHE 22 1812 2091 3045 -197 -88 576 21.720 ATOM 188 CD2 PHE 22 24.290 44.641 1.000 18.62 ANISOU 188 22 2079 CD2 PHE 2106 2890 -143 -623 3 9 4 189 CE1 PHE 22 22.569 21.727 ATOM 46.771 1.000 18.90 ANISOU 189 CE1 PHE 2086 22 1826 3271 -198 -133 3 0 2 ATOM 190 CE2 PHE 22 22.911 21.660 44.379 1.000 19.28 2023 ANISOU 190 CE2 PHE 2189 3114 -242 -754 - 144 22 ATOM 191 CZPHE 22 22.059 21.645 45.473 1.000 19.42 ANISOU 191 CZPHE 22 2048 1723 3607 90 -483 +376 192 27.580 18.971 MOTA N ARG 23 45.583 1.000 17.88 ANISOU 192 1647 N ARG 23 2437 2709 -168 -218 3 1 7 27.520 MOTA 193 CAARG 23 17.594 45.079 1.000 19.18 ANISOU 193 CA 1724 ARG 23 2539 3022 -166 36 158 194 C 46.211 1.000 19.11 MOTA ARG 23 27.767 16.595 ANISOU 194 C 23 1279 ARG 2461 3518 -173 -113 4 5 5 195 0 ATOM ARG 23 27.107 15.547 46.229 1.000 18.82 ANISOU 195 O -33 ARG 23 1614 2156 3381 181 -128 ATOM 196 CB ARG 23 28.605 17.351 44.030 1.000 22.81 ANISOU 196 CB ARG 23 1934 4099 2633 -34 -105 - 354ATOM 197 CG 17.790 42.617 1.000 24.82 ARG 23 28.248 ANISOU 197 2601 -122 - 204СG ARG 23 4078 2752 191 198 17.272 41.685 1.000 29.71 ATOM CDARG 23 29.376 5619 -285 908 704 ANISOU 198 CD ARG 23 2503 3168 199 MOTA ΝE ARG 23 30.479 18.206 41.800 1.000 30.96 ANISOU 199 ARG 2877 286 297 NE 23 5034 3851 -43 ATOM 200 CZARG 30.549 19.360 41.148 1.000 29.49 23 ANISOU 200 CZARG 23 2612 5063 3529 -225 606 177 23 MOTA 201 NH1 ARG 29.536 19.665 40.328 1.000 29.26 331 525 ANISOU 201 NH1 ARG 23 3242 4951 2923 -960 ATOM 202 NH2 ARG 23 31.629 20.092 41.345 1.000 32.61 ANISOU 202 NH2 ARG 4722 -134 519 179 23 2320 5347 MOTA 203 ARG 28.708 16.851 47.125 1.000 17.80 N 24 ANISOU 203 ARG N 24 1262 2168 3332 183 38 9 8 MOTA 204 CAARG 24 28.930 15.899 48.222 1.000 18.85 ANISOU 204 CA ARG 24 1368 2509 3287 69 -162 105 27.701 ATOM 205 ARG 24 15.811 49.114 1.000 17.51 ANISOU 205 ARG C 24 1456 2015 3181 132 -177 2 4 3 MOTA 206 ARG 24 27.333 14.733 49.544 1.000 17.93 0 ANISOU 206 0 ARG 24 1965 -16 -402 2 5 3 1851 2997 24 ATOM 207 СB ARG 30.203 16.321 48.991 1.000 19.88 ANISOU 207 CB ARG 24 1685 2700 3169 -398 -218 4 4 24 MOTA 208 CG ARG 31.459 16.053 48.135 1.000 29.07 ANISOU 208 CG ARG 24 1467 4625 4954 269 203 709 MOTA 32.700 16.206 49.016 1.000 41.84 209 CD ARG 24 ANISOU 209 CD 24 ARG 1745 7021 7130 -451 -494 -922 17.103 48.464 1.000 57.06 MOTA 210 ИΕ ARG 24 33.690 -3326 -669 -1141 ANISOU 210 ΝE ARG 24 4362 9316 8003 ATOM 18.327 48.810 1.000 60.67 211 CZARG 24 34.032 6723 -4627 -1324 -1586 ANISOU 211 CZARG 24 5961 10369 MOTA 212 NH1 ARG 24 33.430 18.980 49.799 1.000 49.70 ANISOU 212 NH1 ARG 24 7748 6565 4569 -951 -2185 2226 ATOM 213 NH2 ARG 24 34.997 18.971 48.159 1.000 54.12 ANISOU 213 NH2 ARG 24 8696 8490 3378 -3780 -2352 1607 MOTA 214 25 N CYS 27.092 16.963 49.370 1.000 15.74

- 20 -

						- 20 -			
ANISOU		N	CYS	25	1435	1969	2574	-16	-393 - 33
ATOM	215	CA	CYS	25	25.884	16.921	50.223	1.000	16.39
ANISOU	215	CA	CYS	25	1518	1954	2756	-95	-317 - 300
ATOM	216	C	CYS	25	24.826	16.068	49.547		15.73
ANISOU	216	Č	CYS	25	1629	1699	2648	-114	-432 6 6
ATOM	217	0	CYS	25					15.89
		_			24.124	15.262	50.155		
ANISOU	217	0_	CYS	25	1453	1801	2783	-88	-469 2 5 2
ATOM	218	СB	CYS	25	25.367	18.362	50.424		
ANISOU		CB	CYS	25	1644	1779	2629	-49	-261 - 30
\mathtt{ATOM}	219	SG	CYS	25	23.700	18.417	51.184	1.000	
ANISOU	219	SG	CYS	25	1742	1825	3202	-122	-33 - 55
ATOM	220	N	LEU	26	24.623	16.308	48.250	1.000	15.25
ANISOU	220	N	LEU	26	1449	1843	2504	-54	-263 -142
ATOM	221	CA	LEU	26	23.560	15.590	47.534	1.000	
ANISOU	221	CA	LEU	26	1616	1739	2580	-86	-453 4 8
ATOM	222	C	LEU	26	23.763	14.085	47.621		
ANISOU		Ċ	LEU	26	1697	1764	2306	-113	-479 6
ATOM	223	0	LEU	26	22.819	13.345	47.771		
ANISOU		0	LEU	26	1797	1725	2920	-234	-664 - 300
ATOM	224	CB	LEU	26	23.526	16.068	46.066		
ANISOU		CB	LEU	26	1811	1645	2633	-191	-483 1 2 2
ATOM	225	CG	LEU	26	23.057	17.510	45.864		
ANISOU	225	CG	LEU	26	1762	1716	2485	-6 -1	
\mathtt{ATOM}	226		LEU	26	23.252	17.880	44.405		
ANISOU			LEU	26	1750	2360	2532	-17	-130 4 6 5
\mathtt{MOTA}	227	CD2	LEU	26	21.584	17.680	46.290	1.000	
ANISOU	227	CD2	LEU	26	1655	2188	2660	-29	-75 168
ATOM	228	N	ARG	27	25.027	13.648	47.494	1.000	17.26
ANISOU	228	N	ARG	27	1870	1818	2871	155	-326 1 4 0
MOTA	229	CA	ARG	27	25.295	12.205			18.75
ANISOU	229	CA	ARG	27	2108	1845	3170	270	-955 1 0 2
ATOM	230	C	ARG	27	25.240	11.599			17.95
ANISOU		Ĉ	ARG	27	1667	1801	3351	159	-897 2 1 9
ATOM	231	Õ	ARG	27	24.777	10.454	48.913		20.99
ANISOU		ŏ	ARG	27	2158	1793	4026	-43	-360 1 6 8
ATOM	232	СВ	ARG	27	26.641	12.008	46.670		21.35
ANISOU		CB	ARG	27	2815	2034	3264	622	-377 - 129
ATOM	233	N	ASP	28	25.827	12.293			
									16.71 -328 6 7
ANISOU ATOM		N	ASP	28	1487	2004	2856	178	
	234	CA	ASP	28	26.034	11.672	51.026		17.47
ANISOU		CA	ASP	28	1613	2095	2931	107	-301 1 2 7
ATOM	235	C	ASP	28	24.872	11.866			17.22
ANISOU		C	ASP	28	1414	2264	2863	223	-447 4 7 1
ATOM	236	0	ASP	28	24.816	11.081			17.62
ANISOU		0	ASP	28	1932	2139	2624	150	-565 3 2 7
ATOM	237	CB	ASP	28	27.306	12.237			22.17
ANISOU		CB	ASP	28	1581	3894	2948	-272	-467 5 5 9
MOTA	238	ÇG	ASP	28	28.590	11.906	50.941	1.000	24.72
ANISOU		CG	ASP	28	1596	3323	4472	236	-288 648
ATOM	239	OD1	ASP	28	28.572	10.905	50.199	1.000	27.56
ANISOU		OD1	. ASP	28	2317	3071	5084	808	-284 5 7 2
ATOM	240		ASP	28	29.573	12.617			32.08
ANISOU			ASP	28	1584	4343	6261	-144	
ATOM	241	N	LYS	29	24.098	12.942			15.57
ANISOU		N	LYS	29	1475	1814	2627		303 178
ATOM	242	CA	LYS	29	23.048	13.305	52 778		15.13
ANISOU		CA	LYS	29	1584	1999	2165	-68	-500 - 96
ATOM	243	C	LYS	29	21.686	13.500			14.56
ANISOU		C	LYS	29	1496	13.300	2686	77 -4	
ATOM	244	0	LYS	29	20.688	12.985	50 625		16.21
ANISOU		0	LYS	29	1627	1876	2657	-177	
11141100		0	ديد	43	1021	10/0	2021	1 1	J . J . J

245 CB LYS 29 23.431 14.563 53.574 1.000 16.09 ANISOU 245 CB LYS 29 1666 1672 2777 3 -642 - 25 MOTA 246 CG LYS 29 24.776 14.421 54.292 1.000 17.68 29 ANISOU 246 CG LYS 2192 1918 2606 7 -1144 1 4 1 CD LYS 29 247 25.161 15.647 55.096 1.000 20.71 MOTA ANISOU 247 CD LYS 29 2675 2044 3151 -35 -1518 4 1 ATOM 248 CE LYS 29 26.498 15.331 55.844 1.000 22.24 ANISOU 248 29 CE LYS 2203 2714 3535 142 -1369 -685 249 ΝZ LYS 29 26.955 16.594 56.492 1.000 32.67 ATOM ANISOU 249 NZLYS 29 3199 3381 5831 -502 -2085 -1260 21.604 14.198 50.993 1.000 14.09 ATOM 250 N GLY 30 ANISOU 250 N GLY 30 1552 1461 2340 135 -455 - 100 251 CA GLY 20.358 14.373 MOTA 30 50.250 1.000 14.09 ANISOU 251 CA GLY 1428 3 0 2365 1561 92 - 342 - 97 252 C GLY ATOM 3 0 19.372 15.284 50.955 1.000 12.30 ANISOU 252 C GLY30 1423 1192 2059 -95 -275 9 4 253 O GLY ATOM 30 18.168 15.223 50.696 1.000 14.58 ANISOU 253 O GLY 30 1435 1689 2415 52 -476 -121 254 N LEU ATOM 31 19.884 16.146 51.823 1.000 13.93 ANISOU 254 N 2343 LEU 31 1472 1479 -182 -248 -181255 CA LEU 31 19.012 17.114 52.511 1.000 14.44 ATOM ANISOU 255 CA LEU 31 1534 1457 2495 -235 -55 -246 256 C LEU 31 19.894 18.286 52.942 1.000 15.08 ATOM ANISOU 256 C LEU 31 1411 1535 2784 -177 -326 - 314 ATOM 257 0 LEU 31 21.113 18.136 53.140 1.000 15.64 ANISOU 257 0 LEU 31 1468 1664 2812 -169 -328 - 67 CB LEU MOTA 258 31 18.222 16.560 53.694 1.000 16.76 CB LEU ANISOU 258 31 2192 1664 2511 -367 128 -213 LEU 18.883 16.517 ATOM259 CG 31 55.039 1.000 20.16 ANISOU 259 CG LEU 2739 -289 -141 4 4 5 31 2485 2435 ATOM CD1 LEU 260 31 17.977 16.145 56.202 1.000 26.49 ANISOU 260 CD1 LEU 31 2253 5076 2738 -508 -341 9 6 9 ATOM 261 CD2 LEU 31 20.052 15.526 55.032 1.000 24.73 ANISOU 261 CD2 LEU 31 4192 2967 2237 1001 153 610 262 N ATOM PHE 32 19.289 19.462 53.052 1.000 14.11 ANISOU 262 N PHE32 1569 1457 2335 -231 -179 - 207 ATOM 263 CA PHE 32 20.020 20.697 53.417 1.000 13.56 ANISOU 263 CA PHE ATOM 264 C PHE 32 1447 2317 1389 -225 -137 1 4 32 18.976 21.777 53.687 1.000 13.72 ANISOU 264 C PHE ATOM 265 O PHE ANISOU 265 O PHE ATOM 266 CB PHE ANISOU 266 CB PHE 32 1411 1439 2365 -218 -421 - 142 32 17.889 21.711 53.118 1.000 15.50 -175 -436 - 389 32 1392 1862 2634 32 20.958 21.157 52.308 1.000 15.01 1379 32 2201 2125 -305 -342 2 3 1 50.920 1.000 14.60 MOTA 267 CG PHE 32 20.381 21.156 CG PHE ANISOU 267 32 1649 1662 2237 -193 -429 1 1 8 CD1 PHE ATOM 268 32 20.326 19.986 50.148 1.000 14.53 ANISOU 268 CD1 PHE 32 1328 1688 2504 -156 -507 1 5 MOTA 269 CD2 PHE 32 19.831 22.345 50.396 1.000 13.66 ANISOU 269 CD2 PHE -179 -309 1 6 6 32 1320 1678 2191 270 ATOM CE1 PHE 32 19.742 20.033 48.892 1.000 14.26 ANISOU 270 CE1 PHE 32 1507 1655 2256 -346 -271 1 9 9 MOTA 271 CE2 PHE 32 19.267 22.348 49.138 1.000 15.49 ANISOU 271 CE2 PHE 32 1681 1932 2272 72 -504 -126 ATOM 272 19.177 21.184 48.385 1.000 15.25 CZPHE 32 ANISOU 272 CZPHE 32 1979 1700 2117 -185 -295 1 6 8 273 N 22.785 54.442 1.000 14.44 ATOM TYR 33 19.376 ANISOU 273 TYR 33 N 2372 -237 -496 - 50 1813 1302 ATOM 274 CA TYR 33 24.023 54.519 1.000 14.32 18.616 1415 ANISOU 274 CA TYR 33 1764 2261 -143 -295 -111 ATOM 275 TYR 33 19.039 24.929 53.364 1.000 13.70

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- 22 -
ANISOU 275
          С
               TYR
                    33
                        1479
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                                        52.859 1.000 15.28
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MOTA
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ANISOU 276
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                                1524
       277
           CB
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ATOM
ANISOU 277
           CB
               TYR
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       278
           CG
               TYR
                    33
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MOTA
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ANISOU 278
           CG TYR
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                        2131
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       279
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MOTA
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           CD2 TYR
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ATOM
ANISOU 280
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                        2901
                                 2070
                                        2468
                                                     115 192
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ATOM
       281
           CE1 TYR
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            CE2 TYR
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MOTA
ANISOU 282
            CE2 TYR
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            CZ TYR
                                        59.263 1.000 22.02
MOTA
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ANISOU 283
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ATOM
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ANISOU 284
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ATOM
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MOTA
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           CA
ANISOU 286
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       287
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            С
                LEU
ATOM
                     34
ANISOU 287
            С
                LEU
                     34
                         1703
                                 1575
                                         2217 -146 -241 -
                         16.716
ATOM
       288
           0
                LEU
                     34
                                 28.289 52.492 1.000 16.95
                         1663
                                 1852
ANISOU 288
                LEU
                     34
                                         2923
                                               -75
                                                      -186 - 64
           0
                                 26.127 50.598 1.000 16.54
       289
           CB
               LEU
                     34
                         17.389
ATOM
ANISOU 289
               LEU
                                                -212 -749 2
            СB
                     34
                         2355
                                 1485
                                         2444
                                 26.800 49.249 1.000 15.65
               LEU
                         17.633
MOTA
       290
            CG
                     34
ANISOU 290
            CG LEU
                         2010
                                 1567
                                         2371
                                               -7 -633 - 63
                     34
                                 26.422 48.664 1.000 20.14
ATOM
       291
            CD1 LEU
                     34
                         18.977
                                                -225 -171 2 6 0
ANISOU 291
            CD1 LEU
                     34
                         1919
                                 2018
                                         3717
                                 26.535 48.291 1.000 17.29
       292
            CD2 LEU
                     34
                         16.490
ATOM
                                                -425 -819 2 1 4
ANISOU 292
            CD2 LEU
                     34
                         2152
                                 1824
                                         2592
                                 28.944 52.065 1.000 15.48
MOTA
       293
            N
                THR
                    35
                         18.842
                                                -230 -200 1 3
ANISOU 293
                    35
                         1817
            N
                THR
                                 1532
                                         2534
                         18.587 30.362 52.324 1.000 17.02
       294
            CA THR
                    35
MOTA
                                                -206 -827 -196
ANISOU 294
            CA THR
                    35
                         2149
                                 1537
                                         2781
                         18.491
                                31.127 51.010 1.000 17.04
ATOM
       295
            C
                THR
                     35
                    . 35
ANISOU 295
                         1895
                                 1693
                                         2887
                                                -149
                                                     -882 - 44
            С
                THR
                                30.572 49.938 1.000 17.01
MOTA
       296
                THR
                     35
                         18.765
            0
ANISOU 296
            0
                THR
                     35
                         1880
                                 1692
                                         2893
                                                -262 -458 1 4 4
                                30.917 53.180 1.000 17.79
MOTA
       297
            CB
               THR
                     35
                         19.772
                     35
                                                     -854 - 200
ANISOU 297
               THR
                                               -87
            CB
                         2018
                                 1942
                                         2800
                     35
                         20.986 30.673 52.474 1.000 21.10
            OG1 THR
MOTA
       298
ANISOU 298
            OG1 THR
                     35
                                         3873 -253 -364 - 402
                         2110
                                 2035
                                30.331 54.567 1.000 20.44
MOTA
       299
            CG2 THR
                     35
                         19.847
                                                      -1113 5 9
ANISOU 299
            CG2 THR
                                         2971
                                                228
                     35
                         2600
                                 2194
MOTA
       300
                     36
                         18.186
                                32.407 51.059 1.000 18.62
            N
                ASP
ANISOU 300
                                                -187 -316 1 4 9
                ASP
                     36
                         2287
                                 1747
                                         3040
                         18.240 33.300 49.884 1.000 20.75
MOTA
       301
               ASP
            CA
                     36
                                         3483 -632 -508 3 7 4
ANISOU 301
            CA
               ASP
                     36
                         2678
                                 1722
       302
                         17.474 32.711 48.703 1.000 20.05
ATOM
            C
                ASP
                     36
ANISOU 302
                                                      -928 4 8 9
            C
                ASP
                     36
                         2104
                                 1929
                                         3586
                                                198
                                         47.540 1.000 21.06
                         17.929 32.685
ATOM
        303
            0
                ASP
                      36
                                 1749
 ANISOU 303
                         2593
                                         3662
                                                -496 -756 1 3 1
             \circ
                ASP
                      36
 ATOM
        304
             CB
                ASP
                      36
                          19.703
                                 33.561
                                         49.500 1.000 22.21
 ANISOU 304
                                                -876 -755 8 0 7
             CB
                ASP
                      36
                          2666
                                  2366
                                         3406
                          20.588 34.192 50.551 1.000 23.05
 MOTA
        305
             CG
                ASP
                      36
 ANISOU 305
            CG
                         2537
                                         4402
                                                -175 -833 - 208
               ASP
                      36
                                 1818
```

306 OD1 ASP 36 20.061 34.886 51.457 1.000 26.16 ANISOU 306 OD1 ASP 36 2981 4860 378 -777 - 381 2100 MOTA 307 OD2 ASP 36 21.824 33.982 50.528 1.000 24.87 -950 -628 ANISOU 307 OD2 ASP 36 2532 1994 4924 -49 48.971 1.000 20.25 308 N CYS 37 MOTA 16.282 32.196 ANISOU 308 N CYS 37 2135 1711 3849 118 -638 - 263 47.902 1.000 20.28 MOTA 309 CA CYS 37 15.463 31.587 1478 ANISOU 309 CA CYS 37 2390 3839 136 -799 - 138 CYS 37 ATOM 310 C 14.078 32.183 47.818 1.000 19.90 ANISOU 310 C CYS 37 2374 1724 3463 214 -711 - 74MOTA 311 0 CYS 37 13.176 31.629 47.156 1.000 22.75 ANISOU 311 CYS 37 0 2569 1984 4091 -12 -1108 1 5 CB 312 CYS 37 15.359 48.083 1.000 22.21 MOTA 30.061 ANISOU 312 СВ CYS 37 2739 1454 4247 194 -477 - 115ATOM 313 SG CYS 37 14.500 29.595 49.596 1.000 22.84 ANISOU 313 CYS 37 SG 2854 3942 -203 -922 1 4 1 1884 ATOM 314 GLY 38 13.855 33.390 48.314 1.000 20.85 N 217 ANISOU 314 NGLY 38 2353 1638 3933 -375 - 42 ATOM 315 CAGLY 38 12.570 34.044 48.194 1.000 23.42 ANISOU 315 CA GLY 38 2233 1874 4790 255 -292 1 6 5 MOTA 316 GLY 38 11.534 33.619 49.217 1.000 23.29 ANISOU 316 C GLY 38 2577 2045 4228 113 -136 -601 ATOM 317 0 GLY 38 10.400 34.091 49.129 1.000 25.58 ANISOU 317 0 GLY 38 2529 3424 3765 214 -96 -264 ATOM 318 N LEU 39 11.894 32.836 50.237 1.000 24.55 ANISOU 318 N LEU 39 2310 2980 4037 119 -46 -364 MOTA 319 CALEU 39 10.938 32.331 51.195 1.000 24.44 ANISOU 319 CALEU 39 2637 2964 3684 -105 175 -946 32.885 52.593 1.000 35.41 MOTA 320 С 11.107 LEU 39 C ANISOU 320 -796 165 -1435 LEU 39 5341 4215 3898 11.784 32.313 53.441 1.000 43.41 MOTA 321 0 LEU 39 39 ANISOU 321 0 LEU 7338 4986 4171 -2639 -1333 -303 ATOM 322 CB LEU 39 10.850 30.810 51.206 1.000 26.48 ANISOU 322 49 -70 - 261 CB LEU 39 2879 4244 2940 ATOM 323 CG LEU 39 10.404 30.097 49.921 1.000 30.21 39 ANISOU 323 CG LEU 4834 2452 4195 258 -1618 - 47428.595 49.972 1.000 24.78 ATOM 324 CD1 LEU 39 10.683 ANISOU 324 CD1 LEU 39 -707 -118 3351 2597 3468 424 39 ATOM 30.407 49.640 1.000 27.50 325 CD2 LEU 8.940 ANISOU 325 CD2 LEU 39 860 -860 - 3234828 2118 3503 40 MOTA 326 N THR 10.365 33.957 52.882 1.000 45.58 40 ANISOU 326 N THR 7392 4849 5077 -520 2852 -1993 40 ATOM CA THR 10.610 34.661 54.136 1.000 32.50 327 ANISOU 327 CA THR 40 999 961 - 558 4224 3732 4393 40 MOTA 328 С THR 9.700 34.177 55.248 1.000 29.68 ANISOU 328 С 294 -1630 THR 40 3175 4204 3898 -116 40 33.556 55.031 1.000 39.75 ATOM 329 0 THR 8.653 ANISOU 329 THR 40 5326 -1079 -301 -1653 0 3930 5847 MOTA 330 CB THR 40 10.641 36.183 53.997 1.000 56.31 ANISOU 330 -1417 1006 - 992 CB THR 40 10586 3758 7052 331 OG1 THR 11.545 36.606 52.946 1.000 68.39 ATOM 40 ANISOU 331 OG1 THR 40 7379 3900 14707 -1978 3617 -246 CG2 THR 11.214 MOTA 332 40 36.837 55.256 1.000 70.22 13188 1389 -4422 -3241 CG2 THR ANISOU 332 40 8265 5228 ASP 10.191 34.302 56.486 1.000 33.20 ATOM 333 41 N 3810 -203 307 -1779 ANISOU 333 Ν ASP 41 3580 5223 CA ASP 41 33.943 57.613 1.000 27.51 334 MOTA 9.329 ANISOU 334 CA ASP 41 2705 3858 91 -253 -1061 3891 MOTA 335 С ASP 41 8.107 34.861 57.660 1.000 33.43 32 547 - 1307 ANISOU 335 С ASP 41 3131 3064 6508 34.469 58.101 1.000 30.76 ATOM 336 0 ASP 41 7.034

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						- 24 -			
ANISOU	336	0	ASP	41	2690	3223	5774	141	-149 - 969
ATOM	337	CB	ASP	41	10.113	34.135	58.915		33.51
ANISOU		CB	ASP	41	4853	4026			-698 - 938
ATOM	338	CG	ASP	41	9.453	33.351	60.039		
ANISOU		CG	ASP	41	3324	5291			-501 - 571
MOTA	339		ASP	41	9.152	32.164	59.780		
ANISOU	339	OD1	ASP	41	4040	4681	4557	-380	824 - 92
ATOM	340	OD2	ASP	41	9.395	33.904	61.161	1.000	86.76
ANISOU	340	OD2	ASP	41	18972	10427	3567	-10425	588 -1858
MOTA	341	N	THR	42	8.272	36.089	57.205		
ANISOU		N	THR	42	3217	3695			5 - 5 8 6
ATOM	342	CA	THR	42	7.198	37.074	57.221		
ANISOU		CA	THR	42	4747	4161			
									-861 - 630
ATOM	343	C	THR	42	6.005	36.640	56.375		
ANISOU		C	\mathtt{THR}	42	3333	4044			157 -1162
\mathtt{ATOM}	344	0	THR	42	4.877	36.606	56.900		
ANISOU	344	0	\mathtt{THR}	42	4048	3603	7128		1059 1224
MOTA	345	CB	THR	42	7.751	38.449	56.815	1.000	37.05
ANISOU	345	CB	THR	42	4526	3763	5788	1021	-677 -1532
ATOM	346	OG1	THR	42	8.831	38.301	55.889		98.08
ANISOU	346		THR	42	16381	13757	7127		7500 - 2318
ATOM	347		THR	42	8.358	39.113	58.047		
ANISOU			THR	42	6097	3613	3997	886	-1119 269
ATOM	348	N N	GLU	43	6.259	36.184			34.64
ANISOU									-275 - 698
	349	N	GLU	43	4208 5.391	3312 35.557	5642 54.192	656	
ATOM		CA	GLU	43					
ANISOU		CA	GLU	43	3527	2886	6120	1199	-883 - 152
ATOM	350	C	GLU	43	4.701	34.300	54.713		
ANISOU		C	GLU	43	3454	4151	8229	225	-1743 953
ATOM	351	0	GLU	43	3.484	34.124	54.605		
ANISOU		0	GLU	43	3375	4041	7222	589	-1417 - 578
MOTA	352	CB	GLU	43	6.278	35.074	53.026		
ANISOU		CB	GLU	43	5991	4098	6901		7 -2137
\mathtt{ATOM}	353	CG	GLU	43	6.658	36.125	52.003		53.42
ANISOU	353	CG	${ t GLU}$	43	5931	6417	7949	-993	1540 -1338
ATOM	354	CD	GLU	43	7.838	36.976	52.429	1.000	50.41
ANISOU	354	CD	GLU	43	4087	7601	7467	-439	2486 -1725
ATOM	355	OE1	. GLU	43	8.024	37.112	53.661	1.000	59.44
ANISOU	355	OE1	GLU	43	7237	7592	7757		1632 -2146
MOTA	356	OE2	GLU	43	8.555	37.476	51.531	1.000	71.33
ANISOU			GLU	43	11550	6344	9207		6267 - 4645
ATOM	357	N	LEU	44	5.511	33.373			27.80
ANISOU		N	LEU	44	2837	2924	4802	-55	-626 -227
ATOM	358	CA	LEU	44	4.926	32.222			27.88
ANISOU		CA	LEU	$\frac{1}{4}\frac{1}{4}$	2207	3379	5009	241	813 - 382
MOTA	359	C	LEU	44	3.886	32.670			34.30
ANISOU		C	LEU	44	1930	4771	6333	-537	776 - 2629
ATOM	360	0	LEU	44	2.781	32.159			33.35
								-840	705 -2397
ANISOU		0	LEU	44	2046	5235	5390		
ATOM	361	CB	LEU	44	5.999	31.394			24.59
ANISOU		CB	LEU	44	2781	3494	3070		0 - 74
ATOM	362	CG	LEU	44	5.592	30.147			31.76
ANISOU		CG	LEU	44	2414	5135	4517	-845	792 1217
ATOM	363		l LEU	44	4.563	29.328		1.000	47.71
ANISOU			l LEU	44	5860	7081	5188		3333 - 2541
ATOM	364		2 LEU	44	6.793	29.259			51.56
ANISOU		CD:	2 LEU	44	6294	3688	9608	1956	2240 1382
ATOM	365	N	LYS	45	4.212	33.712	57.694		41.91
ANISOU	365	N	LYS	45	2865	6802	6256	-1455	381 - 3'5 3 7
ATOM	366	CA		45	3.369	34.195			44.31
ANISOU		CA		45	4768	5427	6639		7 - 2985
					•				

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367 LYS 45 1.981 34.582 58.278 1.000 38.58 -245 1221 -2820 ANISOU 367 С LYS 45 4535 3445 6681 58.902 1.000 39.93 MOTA 368 34.238 0 LYS 45 0.984 ANISOU 368 LYS 4857 6720 \circ 45 3594 262 1634 - 2337 MOTA 369 CB LYS 45 4.038 35.400 59.447 1.000 50.20 ANISOU 369 5561 8569 1081 -447 -3980 CB LYS 45 4944 59.706 1.000 53.07 370 CG LYS 45 3.082 36.546 ATOM ANISOU 370 CG LYS 45 3548 6321 10296 1148 -2094 -4809 ATOM 371 CDLYS 45 3.714 37.922 59.622 1.000 58.29 ANISOU 371 CDLYS 5694 45 4723 11730 1422 -3745 -5024 ATOM 372 CE LYS 45 3.199 38.793 60.761 1.000 65.33 ANISOU 372 CE LYS 45 6294 6898 11629 1072 -3430 -5603 ATOM 373 NZLYS 45 1.713 38.779 60.852 1.000 73.75 -718 -1071 -7436 ANISOU 373 ΝZ LYS 45 6392 9216 12412 374 ATOM N SER 46 1.973 35.341 57.193 1.000 36.94 ANISOU 374 N SER 46 4074 3478 6484 -956 1068 - 2939 375 MOTA CASER 46 0.743 35.856 56.607 1.000 37.61 ANISOU 375 CASER 46 3983 3417 6892 -1335 988 -2335 376 SER 34.702 56.137 1.000 34.45 С -0.137 MOTA46 -1104 1656 -2394 ANISOU 376 C SER 46 3430 3057 6602 377 SER -1.337 34.625 56.449 1.000 29.50 ATOM Ω 46 ANISOU 377 0 SER 3195 2789 5224 -587 1093 -1206 46 378 36.726 55.419 1.000 40.36 MOTA CB SER 46 1.160 ANISOU 378 CBSER 46 4102 3809 7425 -2099 617 -1930 379 37.017 MOTA OG SER 46 0.018 54.630 1.000 43.38 8048 -1261 53 -1863 ANISOU 379 OG SER 46 5005 3431 MOTA 380 N ALA 47 0.493 33.808 55.361 1.000 29.82 ANISOU 380 2173 N ALA 47 5910 -18 809 -1228 3246 54.879 1.000 25.84 ATOM 381 CA ALA 47 -0.208 32.623 ANISOU 381 47 7 630 - 891 CAALA 3566 2106 4148 56.058 1.000 25.02 ATOM 382 С ALA 47 -0.722 31.792 ANISOU 382 С 280 - 280 ALA 47 2591 2344 4572 481 31.381 56.063 1.000 23.19 MOTA 383 0 ALA 47 -1.888ANISOU 383 3597 129 0 ALA 47 2850 2366 318 -1119 53.912 1.000 26.76 CB 0.615 MOTA 384 ALA 47 31.791 ANISOU 384 351 -1134 CB 270 ALA47 2892 2764 4511 ATOM 385 48 0.132 31.529 57.041 1.000 24.64 Ν LYS ANISOU 385 LYS 48 3107 2076 4178 130 -57 -1085 Ν ATOM 386 58.202 1.000 25.83 CALYS 48 -0.186 30.712 ANISOU 386 CALYS 3545 2979 3291 -16 30 -1416 48 MOTA 387 С LYS 48 -1.33731.339 59.003 1.000 28.58 ANISOU 387 129 - 2041 C LYS 48 3373 3344 4144 -354 30.694 59.396 1.000 27.04 388 ATOM 0 LYS 48 -2.310ANISOU 388 419 -634 LYS 0 48 3849 2793 3633 312 389 CB LYS 30.654 59.149 1.000 28.95 ATOM 48 1.035 ANISOU 389 CB LYS 48 3507 3294 4200 -274 -257 -738 29.694 60.313 1.000 32.96 MOTA 390 CG LYS 48 0.775 ANISOU 390 -543 -156 CG LYS 48 4412 3214 4897 113 ATOM 391 CD LYS 48 1.418 30.222 61.570 1.000 39.92 -1278 - 39ANISOU 391 CD LYS 48 5828 4616 4724 705 62.769 1.000 33.67 MOTA 392 29.320 CE LYS 48 1.217 ANISOU 392 CE 1402 -205 - 356 LYS 48 3973 4020 4799 MOTA 393 NZLYS 48 0.731 30.100 63.946 1.000 38.33 ANISOU 393 NZLYS 5230 916 -1039 -1555 48 4516 4816 32.656 59.255 1.000 23.78 MOTA 394 ASP 49 -1.253 N ANISOU 394 N ASP 49 2796 3136 3104 79 -459 -1588 ATOM 395 ASP 49 -2.29833.326 60.006 1.000 24.05 CA ANISOU 395 CA ASP 49 2826 2913 3398 -291 366 -1043 396 MOTA C ASP 49 -3.67933.181 59.366 1.000 24.45 C ANISOU 396 ASP 2721 -220 555 -1454 49 3270 3300 397 ATOM 0 ASP 49 -4.637 32.951 60.082 1.000 27.10

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ANISOU 397 ATOM 398 ANISOU 398 ATOM 399 ANISOU 399 ATOM 400	O ASP 49 CB ASP 49 CB ASP 49 CG ASP 49 CG ASP 49 OD1 ASP 49	-26- 2863 3177 -2.034 34.824 3695 3210 -0.924 35.181 5259 4057 -0.556 34.266		0 3 0 . 3 4 713 - 2 1 7 8 0 3 7 . 1 8 9 - 211 - 2 0 0 7
ANISOU 400 ATOM 401 ANISOU 401	OD1 ASP 49 OD2 ASP 49 OD2 ASP 49	-0.556 34.266 3717 4549 -0.525 36.375 7960 3575	61.904 1.000 4408 -737 61.087 1.000 6875 -927	888 -1727 0 48.45
ATOM 402 ANISOU 402 ATOM 403	N LEU 50 N LEU 50 CA LEU 50	-3.788 33.402 3114 2668 -5.123 33.344	58.059 1.000 3513 374 57.471 1.000) 24.46 200 -1298
ANISOU 403 ATOM 404 ANISOU 404	CA LEU 50 C LEU 50 C LEU 50	2949 2145 -5.679 31.937 3345 2197	3614 161 57.328 1.000	397 - 562
ATOM 405 ANISOU 405 ATOM 406	O LEU 50 O LEU 50 CB LEU 50	-6.878 31.741 3463 2502 -5.254 34.137) 24.96 766 -1181
ANISOU 406 ATOM 407 ANISOU 407	CB LEU 50 CG LEU 50 CG LEU 50	3127 2016 -6.661 34.578 3549 3538	3266 -103 55.807 1.000 3881 961	524 - 757 28.87 825 208
ATOM 408 ANISOU 408 ATOM 409 ANISOU 409	CD1 LEU 50 CD1 LEU 50 CD2 LEU 50 CD2 LEU 50	-7.389 35.082 4567 8556 -6.644 35.642 6971 3395	57.049 1.000 6907 940 54.723 1.000	2929 - 1936 0 41.07
ATOM 410 ANISOU 410 ATOM 411	N VAL 51 N VAL 51 CA VAL 51	-4.801 30.956 3345 2052 -5.293 29.580	5240 -1009 57.138 1.000 2877 -160 57.118 1.000	216 -860
ANISOU 411 ATOM 412 ANISOU 412	CA VAL 51 C VAL 51 C VAL 51	2631 2056 -5.631 29.135 4453 2656	2683 -12 58.533 1.000 2485 -753	173 - 303 25.25 587 - 955
ATOM 413 ANISOU 413 ATOM 414 ANISOU 414	O VAL 51 O VAL 51 CB VAL 51 CB VAL 51	-6.652 28.454 4555 2176 -4.377 28.589	58.725 1.000 2795 -484 56.396 1.000	1185 - 827 0 18.78
ATOM 415 ANISOU 415 ATOM 416	CB VAL 51 CG1 VAL 51 CG1 VAL 51 CG2 VAL 51	2729 1786 -3.152 28.238 3002 1841 -5.147 27.306	2620 -72 57.231 1.000 2918 295 56.021 1.000	-13 -480
ANISOU 416 ATOM 417 ANISOU 417	CG2 VAL 51 N ILE 52 N ILE 52	3112 2337 -4.836 29.500 4514 2471	3708 -511 59.534 1.000 2603 388	355 -846
ATOM 418 ANISOU 418 ATOM 419	CA ILE 52 C ILE 52	-5.205 29.114 3488 3010 -6.498 29.771	60.921 1.000 2765 248 61.355 1.000	0 24.38 19 -509
ANISOU 419 ATOM 420 ANISOU 420 ATOM 421	C ILE 52 O ILE 52 O ILE 52 CB ILE 52	3026 2482 -7.328 29.182 3735 2812	3687 -354 62.071 1.000 3989 -198	614 - 334
ANISOU 421 ATOM 422 ANISOU 422	CB ILE 52 CG1 ILE 52 CG1 ILE 52	-4.016 29.427 3321 4347 -2.853 28.439 3278 5248	61.829 1.00 2815 590 61.510 1.00 3425 741	0 - 785
ATOM 423 ANISOU 423 ATOM 424	CG2 ILE 52 CG2 ILE 52 CD1 ILE 52	-4.293 29.312 3827 6199 -1.930 28.351	63.317 1.00 2750 881 62.710 1.00	0 33.62 150 -1454 0 36.22
ANISOU 424 ATOM 425 ANISOU 425 ATOM 426	CD1 ILE 52 N ASP 53 N ASP 53 CA ASP 53	3956 5082 -6.771 30.992 3479 2878 -8.051 31.646	4722 979 60.913 1.00 2974 165 61.278 1.00	609 - 426
ANISOU 426 ATOM 427 ANISOU 427	CA ASP 53 C ASP 53 C ASP 53	3242 2942 -9.201 30.929 3462 2986	2745 -5 3	55 - 677

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428 0 ASP 53 -10.342 30.836 61.051 1.000 29.73 ATOM ASP 53 3468 ANISOU 428 O 3085 4743 -436 937 -1142 429 CB ASP ATOM 53 -7.964 33.084 60.772 1.000 33.83 ANISOU 429 CB ASP 53 3800 2322 6730 -92 1806 - 933430 CG ASP 53 -9.308 33.758 60.583 1.000 32.05 ANISOU 430 CG ASP 53 4652 2412 5113 172 -302 -1138 431 OD1 ASP 61.486 1.000 43.68 MOTA 53 -9.653 34.524 ANISOU 431 OD1 ASP 53 3661 4686 8248 150 1379 - 3120 432 OD2 ASP 53 -9.950 33.556 59.532 1.000 51.30 ATOM ANISOU 432 OD2 ASP 53 8386 6074 5033 -2062 -1738 922 MOTA 433 N PHE 54 -8.933 30.376 59.413 1.000 25.39 ANISOU 433 N PHE 54 3372 2640 3637 72 71 -1176 434 CA PHE 434 CA PHE MOTA 54 -9.917 29.557 58.704 1.000 24.10 ANISOU 434 54 3015 3264 2876 -366 263 -539 435 MOTA PHE 54 -10.180 28.259 59,456 1.000 24.00 ANISOU 435 С PHE 54 3264 3174 2680 -365 459 - 688 436 0 PHE -11.333 27.893 59.686 1.000 28.19 ATOM 54 ANISOU 436 0 PHE 54 3551 3914 -549 1305 -1130 3246 MOTA 437 CB PHE 54 -9.465 29.273 57.263 1.000 23.62 ANISOU 437 CB PHE 2779 54 3241 2955 -249 218 -434MOTA 438 CG PHE 54 -10.522 28.499 56.461 1.000 27.62 ANISOU 438 CG PHE 54 4712 2945 2838 -694 -636 1 4 -11.729 29.078 MOTA 439 CD1 PHE 54 56.087 1.000 31.38 ANISOU 439 CD1 PHE 4658 3654 -951 -262 -621 54 3613 MOTA 440 CD2 PHE 54 -10.283 27.210 56.033 1.000 30.92 5782 ANISOU 440 CD2 PHE 54 2377 -831 293 -844 3589 CE1 PHE -12.653 28.406 55.307 1.000 44.29 MOTA 441 54 5919 -3066 -2057 1178 55.306 1.000 38.69 ANISOU 441 CE1 PHE 54 5504 5404 ATOM 442 CE2 PHE 54 -11.228 26.503 CE2 PHE 7997 ANISOU 442 54 4412 2289 -2803 155 - 387 CZ PHE -12.424 27.092 54.927 1.000 42.33 ATOM 443 54 ANISOU 443 CZ PHE 54 5992 3787 -4256 54 - 446 6305 444 N PHE 55 -9.126 27.558 59.870 1.000 25.87 ATOM-85 431 -839 ANISOU 444 N \mathtt{PHE} 55 3787 2768 3276 26.310 60.625 1.000 25.69 MOTA 445 CA PHE 55 -9.195 68 763 - 711 ANISOU 445 CA PHE 55 3567 3042 3151 ATOM 446 C 55 -9.929 26.484 61.944 1.000 27.69 PHEANISOU 446 C PHE 55 3357 3961 3205 181 703 - 719 ATOM 447 -10.745 25.670 62.373 1.000 30.08 0 PHE 55 ANISOU 447 0 PHE 55 4046 3217 142 878 - 127 4165 MOTA 448 CB PHE 55 -7.759 25.873 60.932 1.000 25.48 55 PHE 3159 ANISOU 448 CB 2964 835 - 638 3556 117 PHE 55 ATOM 449 CG -7.019 25.242 59.762 1.000 26.31 ANISOU 449 55 3437 CG PHE 3039 3522 -468 1068 -1156 -7.611 24.820 58.590 1.000 27.09 MOTA 450 CD1 PHE 55 ANISOU 450 CD1 PHE 55 3553 3895 2845 -1018 1404 - 658 MOTA 451 CD2 PHE 55 -5.651 25.031 59.935 1.000 31.68 ANISOU 451 CD2 PHE 55 3244 4185 4609 -726 1123 - 2221 CE1 PHE MOTA 452 55 -6.878 24.150 57.621 1.000 23.89 CE1 PHE ANISOU 452 551 - 547 55 -58 3472 2525 3079 MOTA 453 CE2 PHE -4.904 24.433 58.950 1.000 31.74 55 ANISOU 453 CE2 PHE 55 3487 4387 4186 226 337 -2304 -5.514 454 24.004 57.770 1.000 24.23 CZ PHE 5 5 ANISOU 454 CZPHE 55 3706 3312 414 -22 -416 2187 455 MOTA Ν GLU 56 -9.633 27.581 62.629 1.000 30.39 ANISOU 455 GLU Ν 56 3961 5033 2553 -308 520 -1110 MOTA 456 CA GLU 56 -10.222 27.875 63.925 1.000 30.18 ANISOU 456 CA GLU 56 4160 4504 2805 -734 1221 -637 457 MOTA С 56 GLU -11.650 28.401 63.820 1.000 33.50 ANISOU 457 С GLU 56 4324 4124 4280 -535 1489 -892 ATOM 458 56 -12.470 28.149 64.708 1.000 44.44 GLU

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ANISOU 458 0 GLU 56 3864 8872 4150 93 1013 1011 459 СВ GLU 56 -9.403 28.978 64.615 1.000 35.85 ANISOU 459 СВ GLU 56 5037 5109 3475 574 -1821 -221 ATOM 460 CG GLU 56 -8.192 28.508 65.401 1.000 38.63 ANISOU 460 СG GLU 56 4804 7152 2721 -337 763 -1692 ATOM 461 CDGLU 56 29.699 -7.395 65.916 1.000 45.55 ANISOU 461 CD GLU 56 5576 7183 4546 -24 -295 - 2330MOTA 462 OE1 GLU -7.935 30.828 65.888 1.000 55.54 56 ANISOU 462 OE1 GLU 56 7344 7247 6512 586 2570 - 3059 ATOM 463 OE2 GLU -6.246 29.492 66.350 1.000 50.41 56 ANISOU 463 OE2 GLU 56 4050 10497 4606 -1066 1163 -2063 MOTA 464 Ν HIS 57 -11.890 29.289 62.866 1.000 32.20 ANISOU 464 Ν HIS 57 3273 4700 4261 -549 1540 - 670 ATOM 465 CA HIS 57 -13.101 30.078 62.909 1.000 33.38 ANISOU 465 CA HIS 57 3795 4885 4002 -110 1553 - 1239 ATOM 466 C HIS 57 -13.981 29.873 61.697 1.000 32.85 ANISOU 466 С HIS 57 3380 4736 4367 278 1506 - 1797 MOTA 467 0 HIS 57 -15.012 30.533 61.571 1.000 37.09 ANISOU 467 0 HIS 57 3362 4733 5998 276 1087 - 2205 ATOM 468 CB HIS 57 -12.802 31.573 62.976 1.000 37.39 ANISOU 468 CB HIS 57 4327 4959 4922 -193 1402 -1970 ATOM 469 57 -11.981 31.949 CG HIS 64.162 1.000 36.99 ANISOU 469 CG HIS 57 4111 5046 4896 680 1344 - 2319 ATOM 470 ND1 HIS 57 -12.465 31.917 65.453 1.000 38.84 ANISOU 470 ND1 HIS 57 4823 -171 1362 -1598 64.232 1.000 37.91 5090 4844 ATOM 471 CD2 HIS 57 -10.707 32.387 ANISOU 471 CD2 HIS 57 5259 -891 1544 -2828 4197 4947 ATOM 472 CE1 HIS 57 -11.510 32.305 66.275 1.000 40.37 ANISOU 472 CE1 HIS 57 5481 5191 4668 -243 1087 -1361 ATOM 473 NE2 HIS 57 -10.441 32.592 65.552 1.000 35.63 ANISOU 473 NE2 HIS 57 4743 4420 4376 980 799 -1492 ATOM 474 N GLY 58 -13.464 29.068 60.786 1.000 32.06 ANISOU 474 GLY Ν 58 4402 3186 4594 5 1572 -1525 ATOM 475 CA GLY -14.290 28.731 59.627 1.000 35.74 58 ANISOU 475 CA GLY 58 4508 4402 4669 -1129 1877 -1893 ATOM 476 C GLY 58 -15.449 27.859 60.099 1.000 31.52 ANISOU 476 C GLY 58 3317 3688 4969 308 1657 - 593 ATOM 477 0 GLY 58 -15.245 26.952 60.922 1.000 32.66 ANISOU 477 0 GLY 58 4561 4176 3674 -204 624 -1012 MOTA 478 Ν SER 59 -16.632 28.152 59.574 1.000 31.03 ANISOU 478 Ν SER 59 3786 3623 4379 519 1142 - 1442 MOTA 479 CASER 59 -17.823 27.359 59.859 1.000 32.03 ANISOU 479 CA SER 59 3305 3925 4939 757 850 -1188 MOTA 480 С SER 59 -17.763 26.034 59.117 1.000 37.27 ANISOU 480 C 59 SER 3654 4001 6507 0 2065 -1682 MOTA 481 0 SER 59 -16.987 25.858 58.181 1.000 31.23 ANISOU 481 0 SER 59 3027 3655 5184 613 1003 - 1174 ATOM 482 СВ SER 59 -19.077 28.136 59.444 1.000 39.80 ANISOU 482 CB SER 59 3930 5925 5266 1707 -545 - 2846 MOTA SER 59 483 OG -19.252 28.159 58.029 1.000 35.38 ANISOU 483 OG SER 59 3505 4800 5137 355 119 -1624 ATOM 484 N GLU 60 -18.589 25.065 59.507 1.000 46.32 ANISOU 484 GLU 60 5438 6083 6078 -2395 2115 -2700 ATOM 485 CA GLU -18.573 23.801 60 58.754 1.000 34.21 ANISOU 485 CA GLU 60 3381 4798 4818 -960 716 -1238 486 ATOM -19.033 24.055 C GLU 60 57.330 1.000 34.22 ANISOU 486 С GLU 60 4659 3711 4632 455 1378 - 847MOTA 487 0 GLU 60 -18.616 23.437 56.361 1.000 29.91 ANISOU 487 0 GLU 60 3708 3040 4615 -679 2037 -604 MOTA 488 CB GLU 60 -19.390 22.742 59.488 1.000 38.26 ANISOU 488 CВ GLU 60 5012 5567 3958 -1599 748 -1000

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MOTA 489 CG GLU 60 -18.625 22.182 60.678 1.000 42.01 ANISOU 489 CG GLU 60 5470 5439 5055 503 950 - 782490 MOTA CD GLU 60 -17.307 21.528 60.312 1.000 45.34 ANISOU 490 CD GLU 60 4036 7496 5695 -885 1094 - 2276 MOTA 491 OE1 GLU -17.219 20.867 59.264 1.000 49.69 60 ANISOU 491 OE1 GLU 60 5383 6809 -864 1730 -2838 6689 492 OE2 GLU 60 ATOM -16.323 21.659 61.084 1.000 43.62 ANISOU 492 OE2 GLU 60 4677 4974 6924 -1984 109 - 12 ATOM 493 N ALA 61 -19.928 25.028 57.167 1.000 34.26 ANISOU 493 Ν ALA 61 3091 3912 6014 -81 1209 - 1122 CA ALA 61 MOTA 494 -20.408 25.324 55.823 1.000 33.07 CA ALA 61 ANISOU 494 1647 4409 6508 -228 657 -1105 CA ALA 61 C ALA 61 O ALA 61 O ALA 61 CB ALA 61 CB ALA 61 N GLU 62 ATOM 495 -19.314 25.876 54.938 1.000 30.69 ANISOU 495 2053 3742 5866 -59 640 -1066 MOTA 496 -19.138 25.482 53.790 1.000 31.15 ANISOU 496 2754 2893 6189 31 793 -1285 ATOM 497 -21.543 26.336 55.932 1.000 34.43 ANISOU 497 2783 4403 5897 288 1210 - 1650 ATOM 498 -18.568 26.824 55.498 1.000 28.80 62 ANISOU 498 N GLU 2168 3404 5371 -9 915 -964 ATOM 499 62 CA GLU -17.478 27.395 54.704 1.000 26.78 ANISOU 499 CA GLU 62 2339 2374 5461 423 871 -413 ATOM 500 C GLU 62 -16.432 26.330 54.389 1.000 22.61 ANISOU 500 C GLU 62 2569 4402 84 1049 - 376 1621 -15.851 26.316 53.289 1.000 24.41 ATOM 501 0 GLU 62 ANISOU 501 0 GLU 62 2399 2669 4209 -132 801 -548MOTA 502 CB GLU -16.861 28.591 55.429 1.000 32.86 62 ANISOU 502 CB GLU 62 3129 2117 7239 251 2039 - 1358 ATOM 503 CG GLU 62 -17.739 29.834 55.554 1.000 34.69 ANISOU 503 CG GLU 62 2824 2859 7499 916 -95 -1430 MOTA 504 CD GLU 62 -17.274 30.810 56.616 1.000 38.93 CD GLU 62 ANISOU 504 4998 2780 7014 1622 224 -1820 OE1 GLU 62 ATOM 505 -16.861 30.391 57.717 1.000 40.92 OE1 GLU 62 ANISOU 505 4844 3636 7068 1268 34 - 1673 OE2 GLU 62 ATOM 506 -17.324 32.041 56.385 1.000 45.13 OE2 GLU 62 ANISOU 506 7600 2889 6658 -525 1698 -1099 ATOM 63 507 N LYS -16.193 25.431 55.345 1.000 25.20 ANISOU 507 63 N LYS 2470 2380 4723 312 1050 8 CA LYS MOTA 63 63 63 508 -15.214 24.369 55.207 1.000 21.62 CA LYS ANISOU 508 2608 2894 2712 688 349 - 446 ATOM 509 С -15.708 23.397 54.147 1.000 22.42 LYS ANISOU 509 С LYS 63 2930 3038 2549 84 433 - 217 ATOM 510 0 LYS 63 -14.913 23.038 53.289 1.000 24.17 ANISOU 510 0 LYS 63 3340 2354 3491 239 782 - 790 ATOM 511 CB LYS 63 -14.940 23.650 56.534 1.000 24.50 ANISOU 511 CB LYS 63 3411 3057 2842 42 -105 -299 ATOM 512 CG LYS 63 -13.963 24.465 57.381 1.000 27.58 ANISOU 512 63 CG LYS 4640 2792 3045 -302 -465 - 306 63 ATOM 513 CD LYS -13.866 23.937 58.811 1.000 26.09 ANISOU 513 CD LYS 63 3132 3570 3211 305 -575 - 12ATOM 514 CE LYS 63 -12.761 24.695 59.560 1.000 28.96 ANISOU 514 CE LYS 63 4342 3579 3083 -317 -286 - 792 ATOM 515 NZLYS -12.927 24.614 61.030 1.000 35.00 63 ANISOU 515 NZLYS 63 4884 5356 3057 64 - 298 - 817 MOTA 516 -17.007 23.112 54.143 1.000 29.82 N ARG 64 ANISOU 516 N ARG 64 3238 2676 5418 -533 1111 - 1259 MOTA 517 CA ARG 64 -17.521 22.169 53.118 1.000 25.56 ANISOU 517 CA ARG 64 2396 2474 4841 -170 1252 -962 ATOM 518 С ARG -17.417 22.735 51.708 1.000 28.45 64 ANISOU 518 C ARG 64 3022 2681 5106 153 1369 - 562 ATOM 519 0 ARG 64 -17.149 21.981 50.759 1.000 22.57

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						- 30 -			
ANISOU		0	ARG	64	1672	2466		-71	148 - 395
ATOM	520	CB	ARG	64	-18.937	21.809	53.537	1.000	32.48
ANISOU		CB	ARG	64	2669	4144	5526	-809	1483 - 1029
ATOM	521	CG	ARG	64	-19.094		54.189	1.000	45.55
ANISOU		CG	ARG	64	4444	4749	8116		1343 - 153
ATOM	522	CD	ARG	64	-20.557		54.080		59.48
ANISOU		CD	ARG	64	5723	6760		-3977	-2863 2461
ATOM	523	ΝE	ARG	64	-20.759		52.714	1.000	77.63
ANISOU		ΝE	ARG	64	10254	9303	9938		-4193 2666
ATOM	524	CZ	ARG	64	-21.166		51.696	1.000	60.23
ANISOU		CZ	ARG	64	5289	6952	10644	-1128	-4334 501
ATOM	525		ARG	64	-21.424				91.64
ANISOU ATOM	526		ARG	64	18286	5072	11461		-3134 - 75
ANISOU			ARG	64	-21.286				43.67
ATOM	527		ARG	64	3318	4095	9178	-183	-1521 2085
ANISOU		N	ALA	65	-17.624	24.041			26.71
ATOM	528	CA	ALA	65	1907	2770	5472	189	936 - 556
ANISOU		CA	ALA ALA	65 65	-17.522				24.91
ATOM	529	C	ALA	65 65	1798	2379	5288	280	417 - 754
ANISOU		C	ALA	65 65	-16.109				21.81
ATOM	530	0	ALA	65 65	1808	2408	~ · ·	597	155 - 626
ANISOU		0	ALA	65 65	-15.935 2127		48.381		24.13
ATOM	531	СВ	ALA	65	-18.023	3076	3964	224	
ANISOU		CB	ALA	65	3096		50.221		31.78
ATOM	532	N	VAL	66	-15.098	2984	5993	1337	
ANISOU		N	VAL	66	1836	1880	3614		19.29
ATOM	533	ĈA	VAL	66	-13.723	24 167		466	360 - 541 18.17
ANISOU		CA	VAL	66	1636	1653		204	18.17 79 - 487
ATOM	534	C	VAL	66	-13.166				15.18
ANISOU	534	С	VAL	66	1516	1638	2613	120	126 - 571
ATOM	535	0	VAL	66	-11.959	22.623	50.353		
ANISOU	535	0	VAL	66	1567	2071	3060	217	-106 - 317
ATOM	536	СВ	VAL	66	-12.784	25.277	50.437		
ANISOU	536	СВ	VAL	66	2175	1576	3433	183	-135 - 598
\mathtt{ATOM}	537	CG1	VAL	66	-13.139	26.627			20.60
ANISOU			VAL	66	2067	1751	4010	219	593 - 83
ATOM	538		VAL	66	-12.736		51.945		
ANISOU		CG2	VAL	66	2689	2066		102	22 - 603
ATOM	539	N	THR	67	-14.048	21.792	50.343		
ANISOU		N	THR	67	1761	1614	3577	-20	-6 -514
ATOM	540	CA	THR		-13.673	20.403	50.563	1.000	17.18
ANISOU		CA	THR	67	1927	1656	2946	-32	50 - 5 5 6
ATOM	541	C	THR	67	-13.979	19.566	49.332	1.000	16.52
ANISOU		C	THR	67	1763	1742	2773		-467
ATOM	542	0	THR	67	-15.107				18.13
ANISOU		0	THR	67	1750	2211	2929		6 - 3 8 3
ATOM	543	CB	THR	67	-14.373				18.54
ANISOU		CB	THR	67	2202	2014	2827	192	224 - 492
ATOM ANISOU	544		THR	67	-14.060				20.14
ATOM	545		THR	67	2481	2251	2920	-108	155 - 468
ANISOU			THR	67	-13.912	18.364			20.04
ATOM	545	N	THR SER	67 60	2393	2016	3203		6 - 2 3 5
ANISOU		N	SER	68 68	-13.030				16.71
ATOM	547	CA	SER	68	1612	1720	3018	-135	154 - 498
ANISOU		CA	SER	68	-13.281 1508				16.33
ATOM	548	C	SER	68		1631	3065		365 - 561
ANISOU		C	SER	68	-14.223 1194		48.05/		14.85
ATOM	549	0	SER	68	-14.303	1775	2672	-81	197 - 448
ANISOU		Ö	SER	68	1783	1775	2659		16.36
		_		5 0	1100	11/3	2039	-145	192 - 481

ATOM 550 CB SER 68 -11.958 17.303 47.257 1.000 17.84 СВ 1459 647 - 313 ANISOU 550 SER 68 2139 3182 -87 ATOM 551 OG 68 -10.998 18.259 46.904 1.000 17.21 SER ANISOU 551 OG SER 68 1659 1987 2893 -75 364 - 4947.054 1.000 15.89 69 -14.929 16.284 MOTA 552 N PRO ANISOU 552 N 69 1574 PRO 2803 -201 -103 -280 1661 553 CA PRO 69 -15.877 15.182 47.339 1.000 16.42 ATOM ANISOU 553 CA PRO 69 1428 1903 2908 -251 -148 -218MOTA 554 C PRO 69 -15.168 13.889 47.684 1.000 17.22 69 ANISOU 554 С PRO 1633 1578 3331 -199 266 -424 MOTA 555 0 PRO 69 -15.794 12.997 48.287 1.000 18.35 -365 ANISOU 555 0 PRO 69 1815 1760 3399 232 - 376 69 -16.712 15.057 MOTA 556 CB PRO 46.060 1.000 16.75 69 ANISOU 556 СВ 2279 PRO 1354 2733 -360 155 - 729MOTA 557 CG PRO 69 -15.799 15.637 45.008 1.000 16.72 ANISOU 557 CG PRO 69 1553 1971 2827 -359 38 - 452 69 558 PRO -15.059 16.797 ATOM CD 45.681 1.000 17.10 ANISOU 558 -344 CDPRO 69 1918 1804 2776 -119 - 31347.366 1.000 18.07 MOTA 559 N VAL 70 -13.884 13.746 ANISOU 559 Ν VAL 70 1716 1764 3384 -89 292 - 215 560 CA 70 -13.100 12.594 MOTA VAL 47.824 1.000 17.34 ANISOU 560 CAVAL 70 2974 -20 260 - 196 1763 1851 -11.995 13.142 ATOM 561 С VAL 70 48.720 1.000 17.59 ANISOU 561 С VAL 70 2207 2788 -180 159 -142 1686 ATOM 562 0 VAL 70 -11.431 14.186 48.389 1.000 18.59 ANISOU 562 3581 -4 9 152 0 VAL 70 1794 1688 46.724 1.000 18.10 563 CB VAL 70 -12.429 11.757 MOTA ANISOU 563 CB VAL 70 1922 1756 3199 -353 560 -446 CG1 VAL 70 -13.441 10.754 46.213 1.000 20.54 ATOM 564 -369 76 -663 ANISOU 564 70 CG1 VAL 1927 2611 3268 45.642 1.000 17.65 565 CG2 VAL 70 -11.760 12.608 MOTA ANISOU 565 CG2 VAL 70 2379 1806 2520 145 9 ATOM 566 PRO 71 -11.697 12.466 49.815 1.000 16.21 N 1653 ANISOU 566 PRO 71 Ν 1810 2695 -34 464 - 156 MOTA 567 CAPRO 71 -10.839 13.091 50.833 1.000 17.32 ANISOU 567 CAPRO 71 1795 1931 2854 -121 184 - 12 12.804 50.590 1.000 17.67 ATOM 568 C PRO 71 -9.356 ANISOU 568 C PRO 2921 71 1865 1927 46 -57 1 5 6 51.350 1.000 20.57 ATOM 569 0 PRO 71 -8.585 12.223 ANISOU 569 0 PRO 71 2218 3350 424 28 4 7 4 2247 MOTA 570 CB PRO 71 -11.362 12.458 52.117 1.000 19.76 ANISOU 570 CB PRO 71 2976 1862 2668 -347 479 MOTA 571 PRO 71 -11.721 11.056 51.670 1.000 19.08 CG ANISOU 571 CG PRO 71 2838 1805 2608 -267 259 - 234572 -12.323 11.220 50.286 1.000 17.97 MOTA CD PRO 71 PRO ANISOU 572 CD71 1974 2538 -390 451 -167 2314 573 THR 72 -8.894 13.338 49.446 1.000 17.15 ATOM N 72 1677 ANISOU 573 THR 2231 2610 -215 -17 -165 N MOTA 574 CA THR 72 -7.57313.012 48.935 1.000 16.83 ANISOU 574 -134 - 472CATHR 72 1721 1863 2810 -60 MOTA 575 72 -6.490 14.000 49.358 1.000 15.20 C THR -304 163 - 73 ANISOU 575 THR 72 1791 1623 2362 13.729 49.104 1.000 17.49 MOTA 576 0 THR 72 -5.320 -31 -225 ANISOU 576 0 THR 72 1776 1961 2908 -61 MOTA 577 CB 72 -7.533 12.971 47.399 1.000 16.18 THR ANISOU 577 CB THR 2748 -146 -86 -261 72 1552 1848 MOTA OG1 THR 72 -8.091 14.238 47.005 1.000 17.81 578 ANISOU 578 -34 OG1 THR 72 1856 1880 3031 115 -191 579 CG2 THR 72 -8.338 11.816 46.825 1.000 17.49 ANISOU 579 CG2 THR 72 1953 2087 2605 -550 181 -329 -6.877 15.098 49.987 1.000 17.78 ATOM 580 Ν MET 73

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ATOM 611 CA GLY 76 -8.858
ANISOU 611 CA GLY 76 1650
ATOM 612 C GLY 76 -8.602
ANISOU 612 C GLY 76 1584
ATOM 613 O GLY 76 -7.469
ANISOU 613 O GLY 76 1638
ATOM 614 N PHE 77 -9.643
ANISOU 614 N PHE 77 -9.584
ANISOU 615 CA PHE 77 -9.584
ANISOU 615 CA PHE 77 1838
ATOM 616 C PHE 77 1855
ATOM 616 C PHE 77 1855
ATOM 617 O PHE 77 1844
ANISOU 617 O PHE 77 1844
ATOM 618 CB PHE 77 1730
ANISOU 618 CB PHE 77 -10.69
ANISOU 619 CG PHE 77 -10.87
ANISOU 619 CG PHE 77 -10.87
 ATOM 611 CA GLY 76 -8.858 22.532 49.637 1.000 16.67
                                                   2260
                                                               2425
                                                                         -70 199 -612
                                 76 -8.602 22.002 51.036 1.000 16.32
                                                   2014
                                                               2602 -126 268 -347
                                 76 -7.469 21.651 51.370 1.000 16.87
                                 76 1638
                                                               2773 -45 308 -218
                                                   1998
                                 77 -9.643 22.025 51.863 1.000 16.88
                                      1597
                                                   2141
                                                               2675 -7 283 -191
                                      -9.584 21.646 53.274 1.000 17.61
                                      1838
                                                   2196
                                                               2656 109
                                                                                328 -114
                                      -9.776 20.154 53.512 1.000 17.64
                                 77 1855 2248
77 -10 500 77
                                                               2600 -68 243 -185
                               77 -10.589 19.528 52.631 1.77
1844 2488 2594 -183 357 -2
77 -10.698 22.383 53.998 1.000 17.70
77 1730 2515 2480 162 65 -34
77 -10.877 22.081 55.473 1.000 19.61
77 2405 2530 2515 195 261 -1
77 -9.966 22.594 56.395 1.000 22.27
77 2514 3523 2426 431 -23 -1
77 -11.917 21.285 55.941 1.000 21.31
77 3282 2070 2743 36 615 -288
77 -10.116 22.294 57.742 1.000 21.05
                                      -10.589 19.528 52.831 1.000 18.23
                                                               2594 -183 357 -240
                                                               2480 162 65 - 344
 ANISOU 619 CG PHE
                                                               2515 195 261 -516
 ATOM 620 CD1 PHE
 ANISOU 620 CD1 PHE
                                                               2426 431 -23 -527
          621 CD2 PHE
 MOTA
 ANISOU 621 CD2 PHE
ATOM 622 CE1 PHE
ANISOU 622 CE1 PHE
ATOM 623 CE2 PHE
ANISOU 623 CE2 PHE
ATOM 624 CZ PHE
ANISOU 624 CZ PHE
ANISOU 625 N THR
ANISOU 625 N THR
ANISOU 626 CA THR
ANISOU 626 CA THR
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ANISOU 627 C THR
ANISOU 627 C THR
ANISOU 628 O THR
ANISOU 628 O THR
ANISOU 629 CB THR
ANISOU 629 CB THR
 ATOM
         622 CE1 PHE
                                 77 2719 2768
                                                               2510
                                                                          171 221 - 339
                               77 -12.079 20.991 57.300 1.000 25.09
                                77 2967 4120
                                                               2447 -501 625 -826
                                 77 -11.175 21.523 58.207 1.000 23.79
                                 77 2263 3681
                                                               3095
                                                                         -1 376 - 756
                                 78 -9.022 19.631 54.490 1.000 17.64
                                 78 1616
                                                   2161
                                                               2925
                                                                          37 336 1
                                 78 -9.296 18.279 54.983 1.000 18.12
                                 78 1926 2243
                                                               2717
                                                                          -157 624 - 28
                                 78 -9.291 18.316 56.505 1.000 18.66
78 2120 2308 2663 -367 519 -
78 -8.335 18.821 57.095 1.000 21.42
                                                                         -367 519 -288
                                 78 2158 2883 3098 -432 90 1 7 7 7 8 -8.252 17.242 54.521 1.000 21.00
                                                                         -432 90 1 7 7
                                 78 2973 2067 2939 113 428 - 78 -8.027 17.392 53.104 1.000 21.18
 ANISOU 629 CB THR
                                                                                  428 - 574
 ATOM 630 OG1 THR
 ANISOU 630 OG1 THR
                                 78 2544 2671 2833 160 317 - 78 -8.735 15.832 54.800 1.000 26.65
                                                                                 317 - 773
         631 CG2 THR
 ATOM
 ANISOU 631 CG2 THR
                                 78 3759 2227 4141 -275 853 -
79 -10.311 17.804 57.181 1.000 20.36
                                 78 3759
                                                                         -275 853 -618
         632 N GLY
 ATOM
 ANISOU 632 N
                         GLY
                                 79 2669
                                                   2379
                                                               2690
                                                                         -670 630 -144
 ATOM
         633 CA GLY
                                 79 -10.344 17.679
                                                               58.623 1.000 25.96
 ANISOU 633 CA GLY
                                 79 3871 3249
                                                               2745
                                                                          -790
                                                                                  576 375
 ATOM
         634 C GLY
                                 79 -10.029 16.238 59.039 1.000 39.70
 ANISOU 634 C GLY
ATOM 635 O GLY
                                 79 6407
                                                   3542
                                                               5135
                                                                          -1658 -1944 1511
                                 79 -10.623 15.303 58.491 1.000 31.02
 ANISOU 635 O GLY
                                 79 4327
                                                   3187
                                                               4272
                                                                         -404 419 - 75
 ATOM 636 N LEU 80 -9.069 16.055 59.936 1.000 36.07 ANISOU 636 N LEU 80 4380 4536 4788 1381 -564 -
                                                               4788 1381 -564 -835
 ATOM 636 N LEU
ATOM 637 CA LEU
ANISOU 637 CA LEU
ATOM 638 C LEU
ANISOU 638 C LEU
ATOM 639 O LEU
ANISOU 639 O LEU
ATOM 640 CB LEU
ANISOU 640 CB LEU
ANISOU 641 CG LEU
                                80 -8.634 14.713 60.340 1.000 32.52
                                80 3640
                                                   4083
                                                               4632 611 -502 -898
                                80 -9.131 14.311 61.716 1.000 39.82
                         LEU 80 5051
                                                   4652
                                                               5428
                                                                         -128 418 -538
                                80 -9.998 14.963 62.305 1.000 37.05
80 5057 3807 5213 -292 666 8
                                                               5213 -292 666 8 7
                                 80 -7.122 14.580 60.265 1.000 38.36
80 3821 5456 5299 1568 -33 -
80 -6.488 14.753 58.883 1.000 38.27
                                                               5299 1568 -33 -1406
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ANISOU 641 CG LEU 80 3714 5900 4926 725 -288 -2588 642 CD1 LEU 80 -5.007 14.359 58.948 1.000 45.41 ANISOU 642 CD1 LEU 80 2579 8505 -1092 -76 3 6170 ATOM 643 -7.170 13.856 57.854 1.000 40.75 CD2 LEU 8 0 ANISOU 643 CD2 LEU 8.0 4296 5601 5587 872 -1965 - 1793644 N MOTA -6.459 17.442 63.930 1.000 36.72 SER 98 ANISOU 644 N SER 98 3404 6429 4118 -2114 -698 1948 MOTA 645 CA SER -5.629 17.877 62.824 1.000 39.59 98 ANISOU 645 CA SER 98 5376 6031 3635 -449 383 ATOM 646 С SER 98 -6.402 18.372 61.610 1.000 29.89 98 ANISOU 646 C SER 3806 3509 4040 141 640 1204 98 MOTA 647 -7.474 17.856 61.304 1.000 38.27 0 SER 98 ANISOU 647 0 SER 4936 4300 5303 -1107 395 885 98 ATOM 648 CB SER -4.694 16.739 62.358 1.000 44.06 98 98 98 ANISOU 648 CB SER 3175 7425 6141 633 -753 2704 -3.672 17.368 61.583 1.000 46.84 MOTA 649 ΟG SER ANISOU 649 0G SER 3497 6502 7797 95 -408 2418 ATOM 650 -5.829 19.317 60.869 1.000 28.56 N MET 99 ANISOU 650 99 5029 3458 2365 -1080 -550 5 -6.426 19.941 59.700 1.000 21.44 N MET -1080 -550 5 4 6 ATOM 651 CA MET 99 ANISOU 651 CA MET 99 2284 3549 2315 -182 157 132 -5.376 20.229 58.624 1.000 19.16 ATOM 652 C MET 99 ANISOU 652 С MET 99 2306 2382 -433 60 1 3 7 2592 2306 2592 2382 -433 60 13 -4.232 20.575 58.930 1.000 23.34 ATOM 653 0 MET 99 ANISOU 653 0 MET 99 2489 3920 2460 -773 225 -410 -7.164 21.209 60.105 1.000 25.20 ATOM 654 CB MET 99 ANISOU 654 CB MET 99 3172 3375 -572 661 -547 3028 ATOM 655 CG MET 99 -8.481 20.965 60.872 1.000 25.85 ANISOU 655 CG MET 99 3172 3862 2787 -275 739 -782 ATOM 656 SD MET 99 -9.251 22.517 61.389 1.000 32.21 ANISOU 656 SD MET 99 4405 3750 4083 -133 1580 - 568 ATOM 657 CE MET 99 -8.884 22.461 63.145 1.000 76.12 ANISOU 657 CE MET 99 14782 11538 2603 -3321 3478 -3241 MOTA 658 N CYS 100 -5.778 20.094 57.361 1.000 18.85 ANISOU 658 N CYS 100 2434 2443 2285 -160 93 1 9 4 ATOM 659 CA CYS 100 -4.868 20.333 56.234 1.000 18.55 ANISOU 659 CA CYS 100 2251 2380 2418 92 127 2 3 6 MOTA 660 CYS 100 -5.496 21.312 55.228 1.000 16.26 С ANISOU 660 C CYS 100 1826 2031 2321 110 329 2 ATOM 661 100 -6.728 21.308 55.071 1.000 17.69 0 CYS ANISOU 661 CYS 0 100 1741 2395 2586 -69 154 - 104 MOTA 662 CB CYS 100 -4.604 18.982 55.545 1.000 18.46 ANISOU 662 CB CYS 100 2822 2081 2111 98 118 5 1 1 ATOM 663 CYS SG 100 -3.243 18.974 54.329 1.000 22.76 ANISOU 663 CYS SG 100 2622 2968 3058 307 391 1 ATOM 664 N 101 -4.697 22.069 54.498 1.000 17.49 TYR ANISOU 664 TYR 101 1839 N 2473 2332 46 291 2 2 4 101 -5.117 22.874 53.373 1.000 15.38 MOTA 665 CA TYR CA TYR ANISOU 665 101 1946 1939 1960 -50 90 - 262 ATOM 666 101 -4.102 22.594 52.245 1.000 13.65 С TYR ANISOU 666 С TYR 101 1676 1543 1967 -2 -123 -151 ATOM 667 0 TYR 101 -2.896 22.629 52.475 1.000 15.95 ANISOU 667 0 TYR 101 1611 2231 2217 -232 - 212-43 ATOM 668 CB TYR 101 -5.122 24.382 53.739 1.000 19.02 ANISOU 668 CB TYR 101 2816 2082 2328 48 - 519 234 ATOM 669 CG TYR 101 -5.617 25.109 52.498 1.000 17.85 ANISOU 669 CG TYR 101 2084 1895 2804 18 - 26 - 231 ATOM 670 CD1 TYR 101 -6.964 25.134 52.171 1.000 18.25 ANISOU 670 CD1 TYR 101 2042 29 28 - 496 1596 3298 671 CD2 TYR 101 -4.730 25.778 51.658 1.000 17.77 ANISOU 671 CD2 TYR 101 2037 1611 3106 -46 **-**125 - 127

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ATOM 672 CE1 TYR 101 -7.406 25.796 51.036 1.000 19.63 ANISOU 672 CE1 TYR 101 1977 1776 3704 88 -241 -221 50.478 1.000 20.46 673 CE2 TYR 101 -5.147 26.386 101 2060 ANISOU 673 CE2 TYR 2608 3108 239 40 182 674 101 -6.504 26.392 MOTA CZTYR 50.166 1.000 20.29 ANISOU 674 CZTYR 101 2187 2397 3127 -73 -353 - 260 ATOM 675 ОН TYR 101 -6.932 26.995 49.000 1.000 23.34 ANISOU 675 101 2790 ОН TYR 2555 3523 -3 -641 5 2 N 676 22.210 ATOM SER 102 -4.648 51.097 1.000 14.60 ANISOU 676 N SER 102 1618 1890 2041 -61 -109 - 477102 -3.797 ATOM 677 CA SER 21.792 49.980 1.000 14.52 ANISOU 677 CA SER 102 1684 1802 2030 -108 62 - 276 MOTA 678 C SER 102 -4.011 22.670 48.747 1.000 14.99 ANISOU 678 C 102 1545 1790 SER ATOM 679 0 SER 102 -5.167 23.105 ANISOU 679 O SER 102 1589 2342 2425 2 128 - 3 680 CB 102 -4.163 20.340 ATOM SER 49.593 1.000 13.82 ANISOU 680 CB 102 1692 SER 1548 2013 174 681 OG 102 -3.996 19.476 ATOM SER 50.720 1.000 16.06 ANISOU 681 OG SER 102 1886 2066 2153 97 -121 6 3 103 -2.978 22.775 MOTA 682 N MET 47.920 1.000 14.47 ANISOU 682 N MET 103 1568 1724 2206 51 -59 1 5 2 ATOM 683 CAMET 103 -3.102 23.552 46.687 1.000 16.58 ANISOU 683 CA 103 2194 MET 1933 2173 331 -74 253 684 C ATOM MET 103 -2.150 23.013 45.608 1.000 14.41 ANISOU 684 C 103 1598 MET 1793 2083 -202 -210 6 3 ATOM 685 0 103 -1.157 22.347 MET 45.920 1.000 16.24 -23 468 ANISOU 685 O MET 103 1527 2384 2259 -61 ATOM 686 CB MET 46.835 1.000 28.78 103 -2.716 25.004 ANISOU 686 CB MET 103 6537 1318 3081 859 -207 3 6 6 ATOM 687 CG MET 103 -3.258 25.986 47.801 1.000 22.60 ANISOU 687 CG MET 103 2531 2157 3900 -161 -57 -29147.506 1.000 20.60 ATOM 688 SD MET 103 -2.338 27.505 ANISOU 688 SD MET 103 2499 1927 -4 -164 -226 3400 MOTA 689 CE MET 103 -2.587 27.945 45.804 1.000 21.63 ANISOU 689 CE MET 103 2319 2601 3300 209 - 236 308 104 -2.439 MOTA 690 N GLY 23.430 44.378 1.000 15.44 ANISOU 690 GLY 104 1468 2169 Ν 2228 -68 -120164ATOM 691 CAGLY104 -1.511 23.199 43.276 1.000 16.13 ANISOU 691 GLY104 1688 CA2202 2241 42 65 4 6 9 104 -1.583 MOTA 692 C GLY 24.355 42.294 1.000 15.76 ANISOU 692 С GLY 104 1706 1997 2286 -194 3 8 8 -32 MOTA 693 0 GLY 104 -1.987 25.478 42.653 1.000 19.06 144 333 ANISOU 693 0 GLY 104 1953 2032 3256 -71 ATOM 694 N THR 105 -1.151 24.092 41.054 1.000 16.73 ANISOU 694 N THR 105 1685 2385 2287 -375 -55 515 695 CA THR 105 -1.115 25.205 40.094 1.000 17.06 ANISOU 695 105 1725 2390 -231 -148 5 7 7 CATHR 2369 ATOM 696 C THR 105 -2.513 25.631 39.635 1.000 19.55 ANISOU 696 С THR 105 1768 -160 -346 5 2 5 1817 3842 ATOM 697 THR 105 -2.680 26.703 39.059 1.000 22.41 0 ANISOU 697 0 THR 105 2262 2116 4136 -119 -520 8 4 2 ATOM 698 CB THR 105 -0.301 24.857 38.840 1.000 17.57 2877 2038 -394 -343 3 7 7 23.675 38.217 1.000 18.66 ANISOU 698 CB THR 105 1759 105 -0.865 105 2035 MOTA 699 OG1 THR ANISOU 699 OG1 THR 2449 2607 -140 -458 4 1 6 24.590 39.178 1.000 18.95 105 1.155 105 1748 MOTA 700 CG2 THR ANISOU 700 CG2 THR 2853 2601 -105 -248 2 9 6 24.751 MOTA 701 106 -3.507 N ALA 39.741 1.000 16.52 ANISOU 701 2293 NALA 106 1596 2389 -180 -1 2 9 8 ATOM 702 CA ALA 106 -4.846 25.035 39.218 1.000 16.59

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- 36 -
ANISOU 702 CA ALA 106 1692
                                1952
                                       2660
                                              -214 -209 2 4 3
       703
                                       39.923 1.000 17.52
           С
               ALA
                    106 -5.848 24.142
                    106 1651
ANISOU
       703
               ALA
                                1821
                                       3186
                                              26 -66 5 5 5
           0
                    106 -5.479
MOTA
       704
               ALA
                                23.323
                                       40.805 1.000 17.88
ANISOU 704
           0
               ALA
                    106 2038
                                2087
                                       2668
                                              59 -51 3 8 8
       705 CB
              ALA
                    106 -4.862
                                       37.713 1.000 20.31
ATOM
                                24.838
ANISOU 705
           CB ALA
                    106 2331
                                2764
                                       2620
                                              -197 -403 4 4 0
       706 N
               ASP
                    107 -7.149 24.329 39.717 1.000 18.00
ATOM
ANISOU 706 N
               ASP
                    107 1576
                                2208
                                       3057 -77 -120 4 9
       707
           CA ASP
                    107 -8.217 23.535 40.344 1.000 17.46
MOTA
ANISOU 707
            CA
              ASP
                    107 1563
                                2191
                                       2881 -83 -472 3 6 3
                    107 -8.173 23.753 41.859 1.000 17.74
ATOM
       708
               ASP
ANISOU 708
           С
               ASP
                    107 1825
                                2044
                                       2869 447 -269 3 6 2
ATOM
       709
               ASP
                    107 -8.458 22.854 42.650 1.000 18.95
           0
ANISOU 709
               ASP
                                2230
           0
                    107 1994
                                        2974 167 -133 4 0 2
                    107 -8.089 22.044 39.990 1.000 19.62
ATOM
       710
           CB ASP
ANISOU 710
           CB ASP
                    107 2213
                                2300
                                       2942 -394 -727 1 7 3
              ASP
                    107 -8.370 21.842 38.508 1.000 20.81
MOTA
       711
           CG
                                       2862 -138 -532 - 14
ANISOU 711
            CG ASP
                    107 1952
                                3093

    107
    -9.369
    22.369
    37.976
    1.000
    25.84

    107
    2524
    3967
    3327
    222
    -1149

    107
    -7.544
    21.168
    37.844
    1.000
    25.86

ATOM
       712
            OD1 ASP
ANISOU 712
           OD1 ASP
                                        3327 222 -1149 -240
MOTA
       713
           OD2 ASP
ANISOU 713
                    107 3314
           OD2 ASP
                                2989
                                        3523
                                              391 -91 -89
                    108 -7.893 24.962 42.298 1.000 18.18
ATOM
       714 N
               ASN
ANISOU 714 N
                    108 2049
                                                    189 153
               ASN
                                2075
                                        2786 509
ATOM
       715 CA ASN
                    108 -7.831 25.263 43.740 1.000 17.10
ANISOU 715 CA ASN
                    108 1804
                                1977
                                       2715
                                              266
                                                    291 327
ATOM
       716 C
               ASN
                    108 -9.158 25.716 44.314 1.000 17.11
ANISOU 716 C
               ASN
                    108 1705
                                2061
                                        2734
                                              367
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ATOM
       717
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               ASN
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                    108 2066
ANISOU 717
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                                              759
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MOTA
       718
           CB ASN
                    108 -6.799 26.379 43.969 1.000 19.90
                    108 1770
ANISOU 718
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           CB ASN
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                                              186
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ATOM
       719
           CG ASN
                    108 -5.400 25.862 43.717 1.000 17.24
                                       2628
ANISOU 719
           CG ASN
                    108 1709
                                2212
                                              200
                                                     68 1 8 4
       720
                    108 -4.986 24.850 44.277 1.000 17.42
ATOM
           OD1 ASN
ANISOU 720
                    108 2003
           OD1 ASN
                                                     11 - 62
                                1984
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                                               109
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       721
MOTA
           ND2 ASN
ANISOU 721
                    108 2083
           ND2 ASN
                                2326
                                        2587 -82
                                                     300 - 18
MOTA
       722 N
              LEU
                    109 -9.308 25.509 45.607 1.000 18.09
ANISOU 722 N
               LEU
                    109 1795
                                2294
                                        2786
                                              349
                                                     344 1 0
       723 CA LEU
MOTA
                    109 -10.532 25.803 46.369 1.000 19.11
                    109 1763
                                              14 476 - 598
ANISOU 723 CA LEU
                                2200
                                        3296
 ATOM
       724 C
               LEU
                    109 -10.169 26.790 47.457 1.000 17.40
 ANISOU 724
           С
                                                     129 - 207
                LEU
                    109 1682
                                1937
                                        2990
                                               251
               LEU
 MOTA
       725 0
                    109 -9.443 26.423 48.395 1.000 21.18
 ANISOU 725
               LEU
                    109 2443
           0
                                1922
                                       3684
                                              174 -520 2
           CB LEU
                    109 -11.100 24.504 46.940 1.000 17.10
 MOTA
       726
                    109 1888 2142 2469 199 426 -630
109 -11.520 23.425 45.944 1.000 18.07
 ANISOU 726
            CB LEU
 ATOM
       727
            CG
               LEU
               LEU
                     ANISOU 727
            CG
                    109 2515
 ATOM
        728
            CD1 LEU
 ANISOU 728
            CD1 LEU
                     109 2842
                                2406
                                        2375
                                               -331 -175 - 200
                     109 -12.630 23.908 45.035 1.000 25.24
            CD2 LEU
 MOTA
       729
 ANISOU 729 CD2 LEU
                     109 3481
                                2892
                                        3217
                                                     -992 -111
                                               306
 ATOM
       730 N
                PHE
                     110 -10.609 28.036 47.313 1.000 17.25
 ANISOU 730 N
                PHE
                     110 1584 1926
                                        3045
                                               272
                                                     184 - 132
                    110 -10.235 29.071 48.277 1.000 18.20
 MOTA
       731 CA PHE
 ANISOU 731 CA PHE
                    110 1751 1816
                                        3346
                                             169
                                                     221 - 160
       732 C
                     110 -11.409 29.567 49.106 1.000 19.93
                PHE
            С
 ANISOU 732
                PHE
                     110 2077
                              1609
                                        3886
                                               71 650 - 335
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733 0 PHE 110 -12.433 29.948 48.494 1.000 24.64 328 - 779 ANISOU 733 O 110 2051 2461 PHE 4851 612 734 CB PHE 110 -9.607 30.243 47.520 1.000 19.92 110 2367 ANISOU 734 CB PHE 1876 3324 224 619 - 93 CG PHE 110 -8.380 29.986 46.688 1.000 19.47 MOTA 735 ANISOU 735 СG PHE 110 2009 2209 3179 -321 327 - 791 CD1 PHE 110 -7.177 29.680 47.287 1.000 20.59 736 CD1 PHE 110 2071 2080 3674 -274 ANISOU 736 236 737 CD2 PHE 110 -8.437 30.035 45.299 1.000 20.19 MOTA ANISOU 737 CD2 PHE 110 2557 112 1914 3200 543 - 289 110 -6.034 29.454 ATOM 738 CE1 PHE 46.559 1.000 21.06 ANISOU 738 2309 3673 CE1 PHE 110 2020 -386 165 -622 MOTA 739 CE2 PHE 110 -7.277 29.811 44.547 1.000 20.77 ANISOU 739 CE2 PHE 110 2495 2138 3257 197 504 - 398 110 -6.081 29.518 45.175 1.000 22.42 740 CZ PHE 110 2747 2092 3678 531 339 - 357 ANISOU 740 CZPHE 111 -11.238 29.718 50.416 1.000 22.11 ATOM 741 N PRO ANISOU 741 N PRO 111 2250 2153 3996 -72 871 -620 111 -12.287 30.389 51.195 1.000 28.23 ATOM 742 CAPRO 111 3895 ANISOU 742 CA PRO 2210 4621 698 1514 - 671 111 -12.333 31.866 50.784 1.000 30.57 MOTA 743 C PRO ANISOU 743 111 4528 5061 410 410 -1041 С PRO 2026 744 111 -11.390 32.340 50.115 1.000 31.71 ATOM 0 PRO ANISOU 744 111 4040 -179 -597 - 12 2236 5774 0 PRO ATOM 111 -11.799 30.250 52.627 1.000 33.20 745 CB PRO ANISOU 745 CB PRO 111 5609 2702 4303 671 1671 - 790 111 -10.646 29.326 52.647 1.000 26.04 ATOM 746 CG PRO 111 2742 ANISOU 746 CG PRO 3316 3835 -931 1324 - 192 111 -10.161 29.149 51.230 1.000 22.15 MOTA 747 CD PRO ANISOU 747 CD PRO 111 2587 2307 3522 -471 541 -623 748 N 112 -13.337 32.641 51.150 1.000 42.13 ATOM SER 112 7176 ANISOU 748 N SER 2716 6115 2074 1731 - 526 112 -13.368 34.026 50.672 1.000 44.05 ATOM 749 CA SER ANISOU 749 CASER 112 6799 2255 7684 1107 -485 -826 112 -13.262 34.157 49.149 1.000 68.28 MOTA 750 С SER ANISOU 750 112 13632 -1855 -2077 1301 C SER 4498 7812 751 SER 112 -12.347 34.825 48.646 1.000 95.18 ATOM 0 112 15991 ANISOU 751 SER 8747 -4337 -70 1985 0 11425 752 112 -12.493 35.069 51.349 1.000 39.31 ATOM CB SER ANISOU 752 CB SER 112 2247 4535 8153 580 1662 - 1437 ATOM 753 OG SER 112 -11.474 34.624 52.213 1.000 37.49 747 -1152 ANISOU 753 OG SER 112 7213 2453 4579 806 114 -9.515 37.322 49.945 1.000 36.40 MOTA 754 N ASP N ASP 114 3476 2118 8237 1254 403 1484 CA ASP 114 -8.205 37.586 50.600 1.000 30.79 ANISOU 754 MOTA 755 ANISOU 755 CA ASP 114 3503 2856 5340 1229 1240 9 9 6 ATOM 756 C ASP 114 -7.242 36.402 50.648 1.000 26.16 114 2581 2404 4955 601 1114 8 0 4 114 -6.031 36.458 50.338 1.000 25.45 ANISOU 756 С ASP 114 2581 114 2302 2503 4866 -43 602 1 3 1 114 -8.595 37.874 52.075 1.000 43.68 114 7509 2783 6304 1177 MOTA 757 0 ASP ANISOU 757 0 ASP 758 CB ASP MOTA 1157 2727 - 210 ANISOU 758 CB ASP 114 -7.391 38.386 52.835 1.000 46.96 ATOM 759 CG ASP ANISOU 759 114 9259 2517 519 107 CG ASP 3225 5359 760 OD1 ASP 114 -6.487 38.959 52.189 1.000 83.49 -6354 650 -3056 ANISOU 760 OD1 ASP 114 13724 9866 8132 114 -7.370 38.262 54.071 1.000113.59 MOTA 761 OD2 ASP -6984 -159 -2575 ANISOU 761 114 27880 10550 4730 OD2 ASP MOTA 762 PHE 115 -7.831 35.323 51.153 1.000 22.32 N ANISOU 762 PHE 115 2620 3799 2062 204 954 -114 N 763 CA PHE 115 -7.115 34.026 51.183 1.000 22.69

1909 ANISOU 763 CA PHE 115 2765 3947 118 1093 - 187 764 C PHE 115 -6.502 33.754 49.816 1.000 21.49 ANISOU 764 C PHE 115 2146 2316 3702 305 559 - 255 765 0 115 -5.328 33.362 49.758 1.000 20.51 ATOM PHE ANISOU 765 115 2153 0 PHE 2011 3627 323 488 - 158 766 CB PHE 115 -8.096 32.928 51.638 1.000 20.76 MOTA -3 563 - 473 ANISOU 766 PHE 115 2369 1946 CB 3574 PHE 767 CG 115 -7.496 31.590 51.998 1.000 20.23 ATOM CG PHE -155 629 -377 ANISOU 767 115 2369 1854 3463 CD1 PHE 115 -6.915 30.756 51.041 1.000 20.35 MOTA 768 ANISOU 768 CD1 PHE 115 2572 1786 3372 -195 112 - 756 769 31.152 53.309 1.000 21.11 CD2 PHE 115 -7.474 ATOM ANISOU 769 CD2 PHE 115 2802 1932 3287 -113 17 - 689 ATOM 770 CE1 PHE 115 -6.351 29.538 51.325 1.000 21.09 ANISOU 770 CE1 PHE 115 2502 1728 3784 -295 471 -538 771 115 -6.938 29.901 53.623 1.000 27.40 MOTA CE2 PHE ANISOU 771 CE2 PHE 115 5012 1955 3445 444 43 - 572 772 CZ PHE 115 -6.332 29.110 52.655 1.000 24.92 ANISOU 772 CZ PHE 115 3356 1889 4222 50 1519 221 116 -7.301 33.768 48.757 1.000 21.64 773 N GLU ATOM ANISOU 773 N GLU 116 2396 1835 3990 338 261 - 13 116 -6.750 33.424 47.444 1.000 20.90 ATOM 774 CA GLU ANISOU 774 CA GLU 74 1 1 6 ć' MOTA 775 GLU ANISOU 775 C GLU -108 4 4 8 116 -4.544 33.679 46.604 1.000 20.18 776 0 MOTA GLU ANISOU 776 O GLU ATOM 777 CB GLU 116 2209 2147 3312 424 73 1 3 9 116 -7.851 33.561 46.385 1.000 24.22 ATOM ANISOU 777 CB GLU 116 2425 4139 -467 -237 5 1 9 2638 MOTA 778 CG GLU 116 -7.339 33.331 44.980 1.000 23.27 ANISOU 778 CG GLU 116 2425 3952 -7 -494 750 2465 ATOM 779 CD GLU 116 -8.401 33.273 43.910 1.000 25.02 116 2695 ANISOU 779 CD GLU 2703 4107 -510 -739 1509 780 OE1 GLU 116 -9.617 33.306 44.207 1.000 34.83 ATOM -203 -928 1566 ANISOU 780 OE1 GLU 116 2466 4606 6161 116 -8.001 33.030 42.763 1.000 40.92 ATOM 781 OE2 GLU ANISOU 781 OE2 GLU 116 4389 -24 -968 6 9 3 7172 3988 782 N ARG 117 -5.549 35.571 47.300 1.000 20.60 MOTA 117 2299 1811 3718 382 -10 4 117 -4.374 36.374 46.866 1.000 22.65 ANISOU 782 N ARG 117 2299 -10 469 ATOM 783 CA ARG ANISOU 783 CA ARG ATOM 784 C ARG 117 2230 1791 107 153 4586 351 117 -3.163 35.911 47.648 1.000 21.87 ANISOU 784 C 117 2269 179 9 7 ARG 1865 4178 252 785 117 -2.060 35.789 47.102 1.000 22.10 ATOM 0 ARG ANISOU 785 O 117 2197 ARG 2270 3931 216 41 2 0 5 117 -4.682 37.861 47.105 1.000 29.47 786 CB ARG MOTA ANISOU 786 CB ARG 117 2849 6658 259 -555 - 1 1691 787 117 -3.485 38.815 47.046 1.000 40.24 ATOM CG ARG ANISOU 787 CG ARG 117 3905 8818 -819 -1330 -476 2567 788 CD ARG 117 -3.745 40.160 47.716 1.000 52.75 ANISOU 788 CD ARG 117 4698 2848 12496 -595 -1653 -1669 117 -3.934 39.987 49.155 1.000 68.00 ATOM 789 ARG ΝE 1842 - 3441 ANISOU 789 NE ARG 117 8247 4719 12872 422 790 117 -3.166 40.448 50.126 1.000 78.38 MOTA CZ ARG ANISOU 790 CZ ARG 117 13026 5658 11097 283 448 -2498 791 117 -2.097 41.186 49.849 1.000 89.01 ATOM NH1 ARG ANISOU 791 117 14218 8115 -3550 -6761 3577 NH1 ARG 11488 MOTA 792 NH2 ARG 117 -3.479 40.189 51.391 1.000 82.58 ANISOU 792 117 16575 NH2 ARG 2856 11947 2617 2551 - 2095 MOTA 793 NILE 118 -3.334 35.759 48.954 1.000 21.70 ANISOU 793 N 311 118 2319 271 - 314 ILE 1797 4127

- 38 -

794 CA ILE 118 -2.206 35.425 49.810 1.000 20.99 ANISOU 794 CA ILE 118 2546 294 - 470 1624 3805 408 795 C ILE 118 -1.596 34.073 49.475 1.000 18.79 ATOM ANISOU 795 C ILE 118 2222 1534 3384 218 573 - 201 796 0 ATOM ILE 118 -0.409 33.858 49.323 1.000 17.27 ANISOU 796 ILE 118 2194 2707 С 1663 283 351 - 136 797 CB ILE 118 -2.588 35.542 51.293 1.000 22.62 MOTA ANISOU 797 1997 CB ILE 118 2702 3895 276 416 -856 798 CG1 ILE 118 -2.916 36.995 51.700 1.000 27.54 MOTA ANISOU 798 CG1 ILE 118 5077 1801 3587 503 768 - 401 799 CG2 ILE 118 -1.552 34.940 52.206 1.000 23.59 ATOM ANISOU 799 118 3084 2274 CG2 ILE 3606 183 254 -818 118 -3.493 37.115 53.096 1.000 29.35 ATOM 800 CD1 ILE 118 5212 2054 3885 558 1114 -119 -2.454 33.069 49.341 1.000 17.93 119 2378 1605 2828 147 -80 -ANISOU 800 CD1 ILE 3885 558 1114 - 645 ATOM 801 N TRP ANISOU 801 N TRP 2828 147 -80 -2.69 119 -2.035 31.688 49.103 1.000 16.57 CA TRP ATOM 802 CA TRP 119 2126 ANISOU 802 1538 2630 152 -25 - 16 119 -1.575 31.476 47.676 1.000 16.98 803 C ATOM TRP ANISOU 803 C 119 2126 1723 269 -91 -51 TRP 2604 ATOM 804 O ANISOU 804 O 119 -0.700 30.640 47.455 1.000 17.58 TRP 135 181 6 3 TRP 119 1892 1674 3113 119 -3.127 30.690 49.591 1.000 18.32 805 CB TRP ATOM ANISOU 805 CB TRP 119 2156 1789 3014 -34 806 CG TRP 119 -2.934 30.457 51.082 1.000 18.27 MOTA ANISOU 806 CG TRP 119 2208 1711 3025 86 349 5 6 807 CD1 TRP ATOM 119 -3.354 31.273 52.103 1.000 20.36 ANISOU 807 CD1 TRP 119 2624 2029 3083 276 - 153156 CD2 TRP MOTA 808 119 -2.213 29.383 51.683 1.000 18.61 119 2049 2055 2967 134 263 1 119 -2.955 30.773 53.323 1.000 20.55 ANISOU 808 CD2 TRP 263 110 ATOM 809 NE1 TRP NE1 TRP ANISOU 809 119 2471 2229 3109 92 266 - 106 119 -2.260 29.603 53.073 1.000 20.21 CE2 TRP ATOM 810 CE2 TRP ANISOU 810 119 2529 2258 754 297 2893 180 119 -1.576 28.258 51.147 1.000 18.29 CE3 TRP ATOM 811 ANISOU 811 CE3 TRP 119 2258 1714 2977 42 -70 - 20 CZ2 TRP 119 -1.636 28.728 53.981 1.000 21.97 MOTA 812 119 2876 2526 ANISOU 812 CZ2 TRP 2945 384 51 - 106 ATOM 813 CZ3 TRP 119 -0.968 27.375 52.045 1.000 19.35 ANISOU 813 CZ3 TRP 119 2576 2028 2750 187 415 299 119 -1.026 27.618 53.442 1.000 21.67 MOTA 814 CH2 TRP ANISOU 814 CH2 TRP 250 9 7 119 3033 2379 2823 350 815 N 120 -2.129 32.192 46.701 1.000 16.93 MOTA THR ANISOU 815 N THR 120 2023 1833 2577 122 -112 1 8 816 CA THR 120 -1.598 32.086 45.342 1.000 17.85 MOTA ANISOU 816 CA THR С MOTA 817 THR 120 2031 1855 2629 241 -155 1 9 2 120 0.700 31.960 44.674 1.000 18.67 120 1996 1887 3212 389 -131 1 7 7 120 -2.487 32.865 44.344 1.000 18.10 120 1951 2204 2720 28 -93 3 4 5 ANISOU 817 С THR ATOM 818 0 THR ANISOU 818 0 THR CB THR MOTA 819 CB THR ANISOU 819 120 1951 2204 2720 28 -93 3 4 5 120 -3.773 32.238 44.284 1.000 20.49 820 ATOM OG1 THR OG1 THR ANISOU 820 120 1807 2801 3179 59 -363 558 ATOM 821 CG2 THR 120 -1.919 32.803 42.933 1.000 22,46 CG2 THR ANISOU 821 120 2438 3266 2830 475 118 705 121 0.094 33.708 45.956 1.000 18.62 ATOM 822 GLN N ANISOU 822 N 1657 GLN 121 2180 3237 123 -94 213 MOTA 823 CA GLN 121 1.466 34.232 45.993 1.000 18.15 121 2077 3119 77 96 5 2 0 ANISOU 823 CA GLN 1698 ATOM 824 C GLN 121 2.412 33.284 46.718 1.000 17.04

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ANISOU 825
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                                      3645
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           CB GLN
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MOTA
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                   121 2520
121 2.888
ANISOU 826
           CB GLN
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MOTA
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           CG GLN
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                                      46.871 1.000 27.04
ANISOU 827
           CG GLN
                   121 2949
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ATOM
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ANISOU 828
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MOTA
ANISOU 829
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ATOM
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ATOM
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               TYR
                    122 1891
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122 2526
           CB TYR
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ANISOU 835
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           CG TYR
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MOTA
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ANISOU 836
           CG TYR
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                                      2769 255 -147 - 51
ATOM
       837
           CD1 TYR
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                               30.901 51.323 1.000 21.71
ANISOU 837 CD1 TYR
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ATOM
       838 CD2 TYR
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ANISOU 838 CD2 TYR
                   122 2428
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                                            128
                                                  -267 4 6 8
       839
           CE1 TYR
ATOM
                   122 4.680
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ANISOU 839
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MOTA
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ATOM
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      844 CA PHE
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 MOTA
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           CA PHE
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 ATOM
       845 C
               PHE
 ANISOU 845 C
              PHE
                   123 1681
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 MOTA
       846 O PHE
                   123 4.276
 ANISOU 846 O
              PHE
                   123 1703
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 MOTA
       847 CB PHE
                                     2904 209 -148 1
 ANISOU 847 CB PHE
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       848 CG PHE
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 MOTA
                    ANISOU 848
           CG PHE
                    123 2090
            CD1 PHE
 ATOM
       849
                    123 1680 1439 3494 72 -119 -25
123 1.490 27.259 43.513 1.000 18.22
 ANISOU 849
            CD1 PHE
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 ATOM
       850
            CD2 PHE
 ANISOU 850
            CD2 PHE
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            CE1 PHE
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 MOTA
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       852
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                    123 1.722
            CE2 PHE
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 ANISOU 853 CZ PHE
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ATOM 870 CB ARG 125 7.062 32.468 46.851 1.000 20.45
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ATOM 871 CG ARG 125 6.860 33.916 46.344 1.000 28.23
ANISOU 871 CG ARG 125 3178 2007 5542 147 666 -3
ATOM 872 CD ARG 125 6.693 34.891 47.477 1.000 31.76
ANISOU 872 CD ARG 125 3065 2279 6725 -628 1455 ATOM 873 NE ARG 125 6.496 36.221 46.932 1.000 40.81
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 1.000
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- 42 -
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ATOM 903 OG1 THR 128 8.519 30.849 41.162 1.000 19.14

ANISOU 903 OG1 THR 128 2226 2038 3008 195 -23 5 4 5

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ANISOU 904 CG2 THR 128 2107 1329 3793 125 311 6 18

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ANISOU 906 CA ALA 129 1670 1435 2624 -118 -210 - 22

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ATOM 921	CG ARG	131 9.970	24.737	2660 -54 -493 - 9 4 39.251 1.000 16.08
ANISOU 921	CG ARG	131 1703	1695	2711 -13 -647 - 141
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ATOM 924	CZ ARG	131 8.472	27.716	38.413 1.000 31.86
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ATOM 925	NH1 ARG	131 7.467	27.244	39.138 1.000 31.34
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ANISOU 932	N VAL	133 1522	1515	2139 -63 -362 8 6
ATOM 933	CA VAL	133 16.839	24.363	43.689 1.000 14.86
ANISOU 933	CA VAL	133 1902	1566	2179 120 -491 - 27
ATOM 934	C VAL	133 16.923	23.073	42.890 1.000 15.04
ANISOU 934	C VAL	133 1390	1633	2690 -9 -220 -218
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ANISOU 935 ATOM 936	O VAL CB VAL	133 1442 133 16.545	1814	2630 63 -193 - 9 9
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ANISOU 937	CG1 VAL	133 1544	2123	2708 -249 -437 - 81
ATOM 938	CG2 VAL	133 17.766		45.950 1.000 16.51
ANISOU 938	CG2 VAL	133 1769	1942	2561 -61 -831 6 4
ATOM 939	N ALA	134 15.840	22.583	42.270 1.000 13.73
ANISOU 939	N ALA	134 1605	1451	2160 -75 -397 1 8 5
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ANISOU 940 ATOM 941	CA ALA	134 1505	1796	2100 116 -570 - 3 3
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ATOM 943	CB ALA	134 14.535	20.925	41.032 1.000 16.97
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ANISOU 944	N ARG	135 1848	1600	2433 14 -341 - 2
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ATOM 946	CA ARG	135 2139	23.057	
	C ANG	100 10.002	23.03/	JO. JJJ 1.000 XJ. 10

- 44 -

ANISOU 946 C ARG 135 2059 1370 2535 -134 27 1 2 1 38.176 1.000 18.07 947 ARG 135 19.928 22.604 ANISOU 947 ARG 135 2317 2014 2534 256 276 108 135 17.277 ATOM 948 CB ARG 24.586 38.096 1.000 21.96 ANISOU 948 CB ARG 135 3936 1640 2767 -4 -1480 614 ARG 135 17.571 ATOM 949 CG 24.989 36.689 1.000 27.53 135 5112 ANISOU 949 -610 5 9 5 CG ARG 2482 2866 816 950 135 16.930 ATOM CD ARG 26.332 36.393 1.000 23.27 ANISOU 950 135 3548 CD ARG 2428 2865 148 61 1371 MOTA 951 NΕ ARG 135 15.551 26.309 35.928 1.000 22.68 ANISOU 951 NΕ ARG 135 3488 1575 3556 -116 167 297 135 14.520 952 CZATOM ARG 26.858 36.562 1.000 25.90 ANISOU 952 135 3801 CZARG 2165 3874 921 -506 - 179953 135 14.708 27.515 37.702 1.000 23.50 MOTA NH1 ARG 2378 ANISOU 953 135 3582 NH1 ARG 2969 94 137 5 3 2 954 MOTA NH2 ARG 135 13.287 26.758 36.035 1.000 24.30 ANISOU 954 NH2 ARG 135 3520 2441 3272 -101 72 5 8 2 955 GLU 136 19.403 23.533 40.149 1.000 15.76 ATOM ANISOU 955 Ν GLU 136 1897 1696 2396 -178 17 3 1 8 956 GLU 136 20.752 ATOM CA 23.431 40.694 1.000 15.16 ANISOU 956 -97 CAGLU 136 1687 1770 2302 279 140 957 136 21.186 MOTA С GLU 22.001 40.978 1.000 16.74 ANISOU 957 С GLU 136 1535 3122 -148 -172 - 72 1704 MOTA 958 0 GLU 136 22.350 21.637 40.701 1.000 17.42 ANISOU 958 0 GLU 136 1710 1908 2999 7 30 9 2 136 20.957 136 2048 136 20.762 136 2036 ATOM 959 CB GLU 24.284 41.962 1.000 16.64 ANISOU 959 GLU CB 1785 2487 53 11 - 16 25.772 41.718 1.000 17.80 ATOM 960 CG GLU 1714 ANISOU 960 CG GLU 3014 -286 -169 1 1 0 136 21.534 26.269 40.513 1.000 20.92 MOTA 961 \mathtt{CD} GLU 136 2174 -343 70 4 6 9 ANISOU 961 CD GLU 2273 3503 136 22.742 ATOM 962 OE1 GLU 25.987 40.454 1.000 24.97 136 2116 ANISOU 962 OE1 GLU 2434 4938 -494 531 219 ATOM 963 OE2 GLU 136 21.022 27.037 39.672 1.000 24.77 ANISOU 963 OE2 GLU 136 2975 2618 3817 -708 -133 1029 MOTA 964 VAL 137 20.262 21.172 41.450 1.000 15.34 N ANISOU 964 N VAL 137 1681 1696 2453 -108 -287 1 1 3 MOTA 965 CA VAL 137 20.568 19.750 41.647 1.000 15.92 ANISOU 965 CAVAL 137 1755 1802 2493 83 -4 2 1 0 MOTA 966 C VAL 137 20.926 19.086 40.326 1.000 15.86 137 1604 2555 ANISOU 966 С 1869 VAL -38 -35 6 6 MOTA 967 0 VAL 137 21.905 18.308 40.174 1.000 16.70 137 1617 137 19.358 ANISOU 967 0 VAL 2118 2609 72 -151 - 90 MOTA 968 CBVAL 18.990 42.283 1.000 15.35 CB VAL ANISOU 968 137 1729 1663 2440 8 -29 5 137 19.607 CG1 VAL MOTA 969 17.478 42.176 1.000 16.93 ANISOU 969 137 1521 CG1 VAL 1689 -345 9 3223 160 CG2 VAL ATOM 970 137 19.144 19.420 43.724 1.000 15.43 CG2 VAL -277 1 8 5 ANISOU 970 137 1529 2090 2245 -53 971 138 20.149 19.407 39.284 1.000 15.52 ATOM N LEU ANISOU 971 LEU 138 1625 1735 2535 -105 -61 109 Ν 972 LEU 138 20.378 ATOM CA18.881 37.936 1.000 15.74 ANISOU 972 CALEU 138 1576 1862 2543 -71 15 5 1 973 19.396 37.406 1.000 17.42 MOTA C LEU 138 21.721 138 1588 162 - 45 ANISOU 973 C LEU 2119 2912 -87 ATOM 974 0 LEU 138 22.503 18.609 36.846 1.000 19.13 ANISOU 974 0 LEU 138 1878 2406 2985 186 317 6 2 MOTA 975 CB LEU 138 19.211 19.248 36.996 1.000 14.70 ANISOU 975 CB LEU 138 1592 1642 2349 -50 141 190 976 MOTA CGLEU 138 17.883 18.541 37.375 1.000 14.38 ANISOU 976 138 1657 CG LEU 1409 2399 -44 -4 288

- 45 -ATOM 977 CD1 LEU 138 16.774 19.122 36.491 1.000 16.13 ANISOU 977 -218 1 6 8 138 1743 CD1 LEU 2539 1848 128 978 ATOM CD2 LEU 138 17.975 37.156 1.000 17.48 17.027 ANISOU 978 CD2 LEU 138 2185 1435 3021 -107 **-**480 2 8 7 139 21.963 37.548 1.000 17.44 979 N ARG 20.708 ANISOU 979 N ARG 139 1797 2157 2674 -319 238 192 980 ATOM CA ARG 139 23.189 21.319 36.996 1.000 19.06 ANISOU 980 CA ARG 139 2043 2462 2735 -366 482 376 ATOM 981 С ARG 139 24.419 20.734 37.685 1.000 19.72 ANISOU 981 С ARG 139 1797 2600 3097 -518 482 376 ATOM 982 0 ARG 139 25.461 20.432 37.094 1.000 20.70 ANISOU 982 0 ARG 139 2046 2469 3350 -288 607 195 983 CB 139 23.152 22.850 MOTA ARG 37.101 1.000 24.54 ANISOU 983 СВ ARG 139 2525 2403 4396 -402 951 690 36.073 1.000 36.05 ATOM 984 CG ARG 139 23.886 23.665 CG ANISOU 984 ARG 139 6517 2967 4212 -2176 1609 1 4 0 985 CD 139 23.852 25.148 MOTA ARG 36.443 1.000 44.95 ANISOU 985 CD 139 7459 ARG 1902 7716 -242 -1324 1930 ATOM 986 ΝE ARG 139 22.525 25.727 36.547 1.000 43.27 ANISOU 986 NEARG 139 6637 3846 5959 -828 -2173 -698 139 21.821 ATOM 987 CZARG 26.330 35.605 1.000 41.34 ANISOU 987 CZARG 139 5939 4102 5666 497 645 1140 988 ATOMNH1 ARG 139 22.308 26.436 34.376 1.000 44.01 ANISOU 988 NH1 ARG 139 6564 550 1393 3 3 6 4146 6011 ATOM 989 NH2 ARG 139 20.614 26.837 35.833 1.000 45.75 ANISOU 989 NH2 ARG 139 6162 4618 6602 537 1938 2405 ATOM 990 N ALA 140 24.357 20.566 39.009 1.000 18.77 ANISOU 990 N ALA 140 1742 2387 3003 -255 145 6 9 CA ALA CA ALA C ALA ATOM 991 140 25.532 20.169 39.773 1.000 19.53 ANISOU 991 140 1583 2641 3197 -28 38 - 668 992 140 25.932 18.732 ATOM 39.490 1.000 18.96 ANISOU 992 C 140 2018 ALA 2342 2843 -67 76 - 103 993 0 140 27.109 18.335 ATOM ALA 39.626 1.000 21.36 ANISOU 993 O -2 472 - 80 ALA140 1900 2436 3778 ATOM 994 CB ALA 140 25.273 20.345 41.275 1.000 19.74 ANISOU 994 CB ALA 140 1824 2592 3084 35 0 - 360 ATOM 995 N 39.062 1.000 20.32 THR 141 24.958 17.943 ANISOU 995 N THR 141 2014 2209 3498 -115 305 -138 MOTA 996 CA THR 141 25.151 16.530 38.717 1.000 17.15 ANISOU 996 CA 2609 THR 141 1870 2039 61 51 218 MOTA 997 C THR 141 25.269 16.278 37.208 1.000 17.44 ANISOU 997 C 141 1492 THR 2443 2693 21 278 199 36.792 1.000 19.24 MOTA 998 0 THR 141 25.343 15.106 ANISOU 998 0 THR 141 1871 2623 2814 63 579 - 63 MOTA 999 CB THR 141 24.048 15.629 39.290 1.000 16.79 ANISOU 999 CB THR 141 1708 2410 2261 83 164 3 1 1000 OG1 THR ATOM 141 22.788 38.710 1.000 17.18 16.012 ANISOU 1000 OG1 THR 141 1894 141 23.982 2235 2399 5 1 8 -101 -53 1001 CG2 THR 15.734 MOTA 40.807 1.000 17.83 ANISOU 1001 CG2 THR 2377 141 1521 2878 164 -43 1002 N 142 25.361 36.381 1.000 19.69 MOTA GLY 17.301 ANISOU 1002 N GLY 142 2091 2789 -708 302 297 2603 MOTA 1003 CA GLY 142 25.517 17.123 34.923 1.000 19.08 ANISOU 1003 CA GLY 142 1878 2819 2551 128 -163 2 5 5 MOTA 1004 C GLY 142 24.284 16.441 34.313 1.000 18.75 ANISOU 1004 C 2744 GLY 142 1972 2410 0 252 - 117 1005 0 ATOM GLY 142 24.443 15.755 33.315 1.000 22.41 ANISOU 1005 O GLY 142 2432 -161 571 -6802681 3403 1006 N ATOM THR 143 23.093 16.650 34.854 1.000 17.28 ANISOU 1006 N THR 143 1895 2002 2667 67 300 2 4 4 1007 CA ATOM THR 143 21.909 15.932 34.393 1.000 16.88

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ATOM 1009 O THR 143 20.457 17.713 33.764 1.000 20.30

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    ANISOU 1031 CB

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    -143

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    ANISOU 1032 CG
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    MOTA
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    ANISOU 1033 CD
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    MOTA
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     ANISOU 1034 N
                                             ASP
     ATOM
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    ANISOU 1035 CA ASP
                      1036 C
                                            ASP
    ANISOU 1036 C
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11.735 ATOM 1038 CB ASP 146 14.221 28.717 1.000 23.50 ANISOU 1038 CB -653 908 -665 ASP 146 3489 1671 3769 146 13.636 1039 CG ASP 11.508 27.334 1.000 34.15 ANISOU 1039 CG ASP 146 4070 4205 4700 -1004 361 -2386 146 12.393 1040 OD1 ASP 11.521 27.138 1.000 44.73 MOTA 146 3971 9175 ANISOU 1040 OD1 ASP 3849 -2156 683 378 1041 OD2 ASP 146 14.421 11.229 26.397 1.000 44.78 MOTA ANISOU 1041 OD2 ASP 146 4342 8626 -813 289 -2326 4046 147 13.901 14.854 ATOM 1042 N GLY 27.450 1.000 19.28 ANISOU 1042 N GLY 147 2622 2331 2374 -635 -72 113 1043 CA GLY 147 12.916 15.878 27.171 1.000 18.58 MOTA ANISOU 1043 CA GLY 147 2463 2607 1991 -550 -234 - 36 1044 C GLY 147 13.355 17.262 27.590 1.000 18.25 MOTA ANISOU 1044 C GLY 147 2511 2432 1993 -335 -138 6 4 1045 0 GLY 147 12.586 18.183 27.289 1.000 20.74 MOTA ANISOU 1045 O GLY147 2469 2739 2673 -182 -144 2 0 5 ATOM 1046 N GLY148 14.494 17.357 28.286 1.000 17.38 ANISOU 1046 N GLY 148 2237 2174 2191 -462 - 42 - 9028.672 1.000 16.72 MOTA 1047 CA GLY 148 15.027 18.658 ANISOU 1047 CA GLY 148 2308 1789 2255 39 -82 - 77 ATOM 1048 C GLY 148 14.653 19.076 30.085 1.000 13.94 ANISOU 1048 C 148 1517 77 -201 117 GLY 1645 2135 1049 0 GLY 148 13.637 18.634 ATOM 30.694 1.000 16.29 -151 -77 285 ANISOU 1049 O GLY148 1839 2487 1863 1050 N 149 15.431 20.003 30.641 1.000 14.93 ATOM VAL ANISOU 1050 N VAL 149 1624 1780 2269 1 -193 -14 MOTA 1051 CA VAL 149 15.275 20.509 32.017 1.000 14.16 ANISOU 1051 CA VAL 149 1647 1511 2222 92 -195 8 6 ATOM 1052 C VAL 149 13.958 21.218 32.235 1.000 14.37 ANISOU 1052 C VAL 149 1735 -39 1044 2682 83 188 ATOM 1053 0 VAL 149 13.203 20.970 33.163 1.000 14.63 ANISOU 1053 O 1517 VAL 149 1653 2390 -160 -40 107 1054 CB 149 16.439 21.410 32.417 1.000 14.02 MOTA VAL -112 -57 270 ANISOU 1054 CB VAL 149 1745 1530 2052 ATOM 1055 CG1 VAL 149 16.228 22.101 33.752 1.000 16.48 ANISOU 1055 CG1 VAL -153 -305 8 7 149 2360 1709 2193 1056 CG2 VAL 149 17.733 20.614 ATOM 32.482 1.000 17.85 ANISOU 1056 CG2 VAL 149 1618 1937 3226 -59 -52 441 31.371 1.000 15.26 ATOM 1057 N GLU 150 13.634 22.199 ANISOU 1057 N 150 1759 GLU 1328 2711 186 36 2 6 7 31.687 1.000 14.91 1058 CA GLU 150 12.471 23.028 ANISOU 1058 CA GLU 150 1591 1434 2640 93 13 4 1 5 MOTA 1059 C GLU 150 11.182 22.237 31.553 1.000 16.66 ANISOU 1059 C GLU 150 1680 1980 2670 -197 113 199 MOTA 1060 0 150 10.259 22.408 32.379 1.000 15.89 GLU ANISOU 1060 O 29 79 5 8 0 GLU 150 1697 1761 2578 1061 CB MOTA GLU 150 12.531 24.305 30.874 1.000 17.07 ANISOU 1061 CB GLU 150 1925 1337 189 513 3223 254 150 13.761 25.167 ATOM 1062 CG GLU 31.220 1.000 19.00 ANISOU 1062 CG 150 2483 3523 GLU 1212 -65 -95 32.658 1.000 20.32 ATOM 1063 CD GLU 150 13.810 25.624 ANISOU 1063 CD 150 2444 GLU 1746 3532 -130 -24 1064 OE1 GLU 150 12.781 25.749 33.377 1.000 20.88 ATOM ANISOU 1064 OE1 GLU 150 2558 1728 3648 29 58 3 9 6 1065 OE2 GLU 150 14.913 33.161 1.000 21.77 MOTA 25.946 -165 -202 2 7 3 ANISOU 1065 OE2 GLU 150 2549 3693 2030 1066 N 151 11.050 ATOM ALA 21.288 30.603 1.000 14.98 151 1649 ANISOU 1066 N ALA 1710 2334 37 - 307 551 1067 CA ALA 151 9.834 20.475 30.543 1.000 15.79 ANISOU 1067 CA -173 -198 4 0 8 ALA 151 1820 2045 2136 MOTA 1068 C ALA 151 9.748 19.531 31.724 1.000 15.38

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ANISOU 1068 C ALA 151 1674 1953 2216 165 181 4 4 ATOM 1069 O ALA 151 8.642 19.186 32.184 1.000 16.51 ANISOU 1069 O ALA 151 1778 1852 2643 -152 110 3 3 ATOM 1070 CB ALA 151 9.823 19.663 29.236 1.000 18.05 ANISOU 1070 CB ALA 151 1910 2811 2139 -275 -316 1 6 ATOM 1071 N PHE 152 10.893 19.135 32.306 1.000 14.25 ANISOU 1071 N PHE 152 1858 1132 2423 10 -107 26 3 ATOM 1072 CA PHE 152 10.893 18.285 33.493 1.000 13.42 ANISOU 1072 CA PHE 152 1457 1291 2353 -102 -34 30 ATOM 1073 C PHE 152 10.406 19.056 34.695 1.000 13.93 ANISOU 1073 C PHE 152 1481 1400 2412 -43 -165 19 181 442 -152 110 330 -275 -316 1 6 6 -102 -34 304 1400 2412 -43 -165 1 18.495 35.558 1.000 14.50 152 1481 -165 1 9 6 ATOM 1074 0 PHE 152 9.679 ANISOU 1074 0 PHE 152 1590 1482 2438 25 2 6 -85 1075 CB PHE 152 12.309 17.744 33.728 1.000 13.95 ANISOU 1075 CB PHE 152 1504 1547 2248 -29 111 463 1076 CG PHE 152 12.475 16.966 35.011 1.000 14.04 ATOM ANISOU 1076 CG PHE 152 1747 1386 2200 88 -58 2 4 7 ATOM 1077 CD1 PHE 152 12.032 15.653 35.076 1.000 13.90 ANISOU 1077 CD1 PHE 152 1906 1306 2069 165 -36 2 -36 281 ATOM 1078 CD2 PHE 152 13.094 17.499 36.127 1.000 15.67 ATOM 1078 CD2 PHE 152 13.094 17.499 30.127 1.000 15.07 ANISOU 1078 CD2 PHE 152 1927 1770 2259 -155 -115 2 3 3 ATOM 1079 CE1 PHE 152 12.213 14.949 36.263 1.000 14.06 ANISOU 1079 CE1 PHE 152 1669 1507 2165 182 -282 3 4 7 ATOM 1080 CE2 PHE 152 13.323 16.799 37.276 1.000 14.83 ANISOU 1080 CE2 PHE 152 1724 1671 2240 35 -112 165 ATOM 1081 CZ PHE 152 12.861 15.522 37.361 1.000 14.86 ANISOU 1081 CZ PHE 152 1994 1734 1916 -162 99 113 ATOM 1082 N LEU 153 10.789 20.324 34.789 1.000 15.25 ANISOU 1082 N LEU 153 1742 1355 2696 58 110 15 4 ATOM 1083 CA LEU 153 1742 1355 2696 58 110 15 4 ATOM 1083 CA LEU 153 1742 1355 2696 58 110 15 4 ATOM 1083 CA LEU 153 1742 1355 2696 58 110 15 4 ATOM 1084 C LEU 153 1732 1402 2354 -66 16 20 3 ATOM 1084 C LEU 153 1732 1402 2354 -66 16 20 3 ATOM 1085 O LEU 153 1732 1402 2362 -80 76 1 1 ATOM 1085 O LEU 153 1940 1454 21.151 36.953 1.000 15.82 ANISOU 1086 CB LEU 153 1940 1454 22.216 36.953 1.000 15.82 ANISOU 1086 CB LEU 153 1940 1454 22.216 36.953 1.000 16.53 ANISOU 1086 CB LEU 153 12.914 21.685 36.514 1.000 16.53 ANISOU 1087 CG LEU 153 1893 2013 2135 -33 -186 - 36 ATOM 1088 CD1 LEU 153 13.992 22.829 36.614 1.000 18.41 ANISOU 1088 CD1 LEU 153 1732 2473 2791 -156 80 -876 ANISOU 1078 CD2 PHE 152 1927 1770 2259 -155 -115 2 3 3 2616 -313 312 -157 ANISOU 1088 CD1 LEU 153 1732 2473 2791 -156 80 -876 1089 CD2 LEU 153 12.863 20.883 37.794 1.000 21.76 ATOM ANISOU 1089 CD2 LEU 153 3083 3182 2005 365 261 1 ATOM 1090 N ASP 154 8.473 21.866 34.708 1.000 14.41 2005 365 261 193 ANISOU 1090 N 1090 N ASP 154 1768 1181 2525 -25 -8 29 3 1091 CA ASP 154 7.092 22.373 34.553 1.000 15.90 -25 -8 2 9 3 ATOM ANISOU 1091 CA ASP 154 1665 1615 2760 -195 27 7 6 9 ASP 154 1665 1615 2760 -195 27 76 9

ASP 154 6.216 21.161 34.814 1.000 14.66

ASP 154 1859 1304 2409 -92 143 5

ASP 154 5.995 20.368 33.889 1.000 17.30

ASP 154 2561 1455 2557 -29 314 2

ASP 154 6.923 22.909 33.125 1.000 18.59

ASP 154 1905 2077 3081 124 269 13

ASP 154 5.461 23.157 32.768 1.000 19.87

ASP 154 2029 2531 2990 226 129 14

ASP 154 4.561 23.253 33.639 1.000 19.68

1 ASP 154 1949 2209 3318 92 221 4 9 6 ATOM 1092 C ANISOU 1092 C 143 515 ATOM 1093 0 AN1SOU 1093 O ASP ATOM 1094 CB ASP ANISOU 1094 CB ASP ATOM 1095 CC 314 234 269 1317 1095 CG ASP ATOM ANISOU 1095 CG ASP 129 1436 MOTA 1096 OD1 ASP ANISOU 1096 OD1 ASP 154 1949 2209 3318 92 221 4 9 6 154 5.207 23.189 31.554 1.000 23.73 1097 OD2 ASP ATOM ANISOU 1097 OD2 ASP 154 2512 3475 3029 246 -137 653 155 5.831 20.904 36.070 1.000 14.25 1098 N CYS ANISOU 1098 N CYS 155 1708 1365 2342 -101 -62 546

ATOM 1099 CA CYS 155 5.418 ANISOU 1099 CA CYS 155 1608 ATOM 1100 C CYS 155 1608 ATOM 1100 C CYS 155 1608 ATOM 1101 O CYS 155 1631 ANISOU 1101 O CYS 155 3.224 ANISOU 1101 O CYS 155 1631 ANISOU 1101 O CYS 155 1631 ANISOU 1102 CE CYS 155 6.664 ANISOU 1102 CE CYS 155 6.664 ANISOU 1103 SG CYS 155 7.265 ANISOU 1103 SG CYS 155 1561 ANISOU 1104 N GLU 156 1575 ANISOU 1104 N GLU 156 1575 ANISOU 1105 CA GLU 156 1575 ANISOU 1106 C GLU 156 1575 ANISOU 1107 O GLU 156 1508 ANISOU 1108 CB GLU 156 1508 ANISOU 1109 CG GLU 156 1875 ANISOU 1100 CG GLU 156 1874 ANISOU 1100 CG							- 49 -		
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	ATOM						1434 21.963		

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ANISOU 1129 CA LEU 159 1438 159 0.419 1555 2095 -36 -80 -91 1130 C ATOM LEU 21.494 49.602 1.000 14.49 ANISOU 1130 C LEU 159 1336 2034 2135 -152 -208 -159 -0.790 21.596 49.419 1.000 15.09 2034 -152 -208 - 38 1131 0 ATOM LEU 159 1414 159 1.390 159 1720 ANISOU 1131 O LEU 1999 2319 90 -131 9 0 23.466 48.394 1.000 15.28 1132 CB LEU ANISOU 1132 CB LEU 1447 2639 55 -325 -197 24.320 49.669 1.000 17.11 159 1.484 1133 CG LEU ANISOU 1133 CG LEU 159 2146 1689 2665 363 -332 - 343MOTA 1134 CD1 LEU 159 2.775 24.114 50.453 1.000 18.70 ANISOU 1134 CD1 LEU 159 2276 1759 3070 379 -687 -540 25.801 49.291 1.000 21.00 ATOM 1135 CD2 LEU 159 1.312 ANISOU 1135 CD2 LEU 159 2918 1535 3526 439 -692 - 382 1136 N ARG ATOM 160 0.916 21.107 50.774 1.000 14.37 ANISOU 1136 N ARG 160 1688 1709 2063 -101 -186 4 7 ATOM 1137 CA ARG 20.747 51.901 1.000 15.61 160 0.055 ANISOU 1137 CA ARG 160 1726 1990 2217 -64 90 - 118 ATOM 1138 C ARG 160 0.480 21.501 53.155 1.000 15.40 ANISOU 1138 C ARG 160 1557 2158 2135 -34 -46 -38 ATOM 1139 0 ARG 160 1.639 21.401 53.576 1.000 16.32 ANISOU 1139 O ARG 160 1528 2508 2164 63 41 - 104 ATOM 1140 CB ARG 160 0.048 19.263 52.227 1.000 16.13 ANISOU 1140 CB ARG 160 2134 2084 1912 -127 -30 129 ATOM 1141 CG 160 -0.594 18.410 51.155 1.000 17.17 ARG ANISOU 1141 CG ARG 160 1963 1934 2628 -140 -212 - 60 MOTA 1142 CD 160 -0.672 16.959 51.627 1.000 18.16 ARG 160 2767 1965 2166 125 -330 - 3 160 -1.382 16.102 50.682 1.000 18.11 160 2408 1775 2699 -56 -308 2 0 160 -1.221 14.789 50.581 1.000 16.76 ANISOU 1142 CD ARG -330 - 35 ATOM 1143 NE ARG ANISOU 1143 NE ARG ATOM 1144 CZ ARG 160 2191 1748 2428 -97 55 17 160 -0.326 14.192 51.374 1.000 20.55 ANISOU 1144 CZ ARG 55 1 7 4 ATOM 1145 NH1 ARG 160 2306 2012 3491 -26 -457 3 0 5 160 -1.908 14.095 49.689 1.000 19.23 ANISOU 1145 NH1 ARG MOTA 1146 NH2 ARG ANISOU 1146 NH2 ARG 160 2502 2031 2774 181 -147 - 3 3 8 161 -0.469 22.257 53.755 1.000 15.36 160 2502 ATOM 1147 N PHE 161 1604 2120 2111 -37 -63 -128 161 -0.209 22.975 54.999 1.000 16.25 ANISOU 1147 N PHE ATOM 1148 CA PHE ANISOU 1148 CA PHE 161 2173 1774 2227 -71 -187 - 8 9 ATOM 1149 C 161 -1.030 22.236 56.069 1.000 16.98 PHE ANISOU 1149 C PHE161 1980 2432 2041 -217 -161 -162 MOTA 1150 0 PHE161 -2.248 22.113 55.948 1.000 20.38 ANISOU 1150 O PHE 161 1981 3291 2473 -190 -191 - 72 1151 CB PHE 161 1981 3291 2473 -190 -191 1151 CB PHE 161 -0.683 24.431 54.862 1.000 19.76
1151 CB PHE 161 2065 1903 3540 167 355 -1
1152 CG PHE 161 -0.379 25.259 56.109 1.000 23.61
1152 CG PHE 161 3026 1905 4041 836 -59 -1
1153 CD1 PHE 161 -1.194 25.304 57.228 1.000 28.25
1153 CD1 PHE 161 3992 2474 4268 1077 369 -1 MOTA ANISOU 1151 CB PHE 355 - 198 MOTA ANISOU 1152 CG PHE -59 -591 MOTA ANISOU 1153 CD1 PHE 1077 369 -1253 161 0.807 25.978 56.141 1.000 26.62 ATOM 1154 CD2 PHE 161 4015 ANISOU 1154 CD2 PHE 2483 3616 -130 -927 -106 1155 CE1 PHE 161 -0.850 25.992 58.383 1.000 35.29 ATOM ANISOU 1155 CE1 PHE 161 6873 161 1.153 161 4643 2097 4437 1538 -135 -1399 ATOM 1156 CE2 PHE 26.723 57.258 1.000 33.63 ANISOU 1156 CE2 PHE 3240 4894 1263 -2085 -1268 1157 CZ PHE 161 0.320 26.726 58.363 1.000 36.44 ANISOU 1157 CZ PHE 161 6071 4282 3493 1455 -2477 -1044 162 -0.358 21.767 57.130 1.000 17.59 ATOM 1158 N ARG ANISOU 1158 N ARG 162 2095 2487 2103 -118 -135 - 69 162 -1.072 21.078 58.199 1.000 18.27 162 2769 2414 1758 6 178 - 3 7 8 ATOM1159 CA ARG ANISOU 1159 CA ARG

ATOM 1160 C ARG 162 -0.880 21.758 59.553 1.000 20.16 ANISOU 1160 C ARG 162 2110 3341 2210 -36 1161 0 ARG 162 0.217 22.160 59.893 1.000 19.61 ANISOU 1161 O ARG 162 2257 2993 2201 -194 -73 -359 1162 CB ARG 162 -0.580 19.640 58.356 1.000 20.81 MOTA ANISOU 1162 CB ARG 162 2958 2275 2675 -129 6 -169 1163 CG ARG 162 -0.843 18.724 57.166 1.000 19.90 ATOM ANISOU 1163 CG ARG 162 3044 2073 2443 -112 254 - 38 1164 CD ARG 162 -0.182 17.383 57.393 1.000 28.02 ATOM 162 5599 ANISOU 1164 CD ARG 2038 3010 381 -14 114 ATOM 1165 NE ARG 162 -0.369 16.420 56.326 1.000 27.74 ANISOU 1165 NE ARG 162 4151 2294 4097 555 -687 - 434 1166 CZ ARG 162 -1.278 15.445 56.370 1.000 31.11 MOTA ANISOU 1166 CZ ARG 162 2560 3729 5531 470 -350 - 11521167 NH1 ARG 162 -2.092 15.324 MOTA 57.403 1.000 42.97 ANISOU 1167 NH1 ARG 162 3475 5906 6946 -579 1019 -2492 1168 NH2 ARG 162 -1.329 14.603 55.353 1.000 29.64 ATOM 162 3066 2738 ANISOU 1168 NH2 ARG 5458 120 -143 - 708ATOM 1169 N TYR 163 -1.956 21.780 60.311 1.000 19.52 2901 147 263 - 763 ANISOU 1169 N TYR 163 2394 2120 1170 CA TYR 163 -1.943 22.102 61.732 1.000 22.74 ATOM ANISOU 1170 CA TYR 163 3312 3107 2219 369 302 - 878ATOM1171 C TYR 163 -2.037 20.800 62.536 1.000 24.20 ANISOU 1171 C TYR 3901 2492 -222 253 -189 163 2802 ATOM 1172 0 TYR 163 -2.992 20.049 62.274 1.000 28.02 ANISOU 1172 O TYR 163 2305 4409 3934 -202 -126 3 9 9 TYR 1173 CB MOTA 163 -3.198 22.912 62.114 1.000 28.98 ANISOU 1173 CB TYR 163 3861 1196 - 1783 3231 3920 267 ATOM 1174 CG TYR 163 -3.342 22.997 63.623 1.000 25.58 ANISOU 1174 CG TYR 163 2572 3382 3767 543 749 - 1204163 -2.458 23.826 64.319 1.000 37.32 1175 CD1 TYR ATOM ANISOU 1175 CD1 TYR 163 3654 4413 -759 884 -2373 6112 1176 CD2 TYR 163 -4.315 22.333 64.345 1.000 29.13 ATOM 1084 - 769 ANISOU 1176 CD2 TYR 163 2622 3994 4452 749 1177 CE1 TYR 163 -2.546 23.966 65.702 1.000 38.28 MOTA ANISOU 1177 CE1 TYR 163 2905 -454 987 -2740 7138 4503 1178 CE2 TYR 163 -4.396 22.431 65.726 1.000 37.36 ANISOU 1178 CE2 TYR 163 3220 6336 4640 -273 1997 -1618 ATOM 1179 CZ TYR 163 -3.500 23.250 66.393 1.000 49.85 ANISOU 1179 CZ TYR 163 5272 8795 4872 -1810 1593 -2223 1180 OH TYR ATOM 163 -3.595 23.365 67.768 1.000 44.81 -222 270 -496 ANISOU 1180 OH TYR 163 5246 4413 7368 ATOM 1181 N PHE 164 -1.098 20.651 63.448 1.000 24.84 ANISOU 1181 N 164 2905 PHE 3368 3164 -89 -125 - 361 ATOM 1182 CA PHE ANISOU 1182 CA PHE 164 -1.045 19.532 64.370 1.000 28.14 164 3538 3957 3195 223 -163 - 30MOTA 1183 C PHE 164 -1.360 20.003 65.787 1.000 26.67 ANISOU 1183 C -194 - 257PHE 164 2964 3937 3234 -473 164 -0.540 MOTA 1184 0 PHE 20.730 66.342 1.000 31.26 ANISOU 1184 O 164 3119 -959 -260 -519 PHE 4888 3869 1185 CB PHE 164 0.347 18.881 64.396 1.000 27.86 MOTA ANISOU 1185 CB PHE 164 3423 3725 3436 76 -199 164 0.744 18.301 63.052 1.000 26.77 1186 CG PHE 3474 ANISOU 1186 CG PHE 164 2914 3785 -598 74 - 275 MOTA 1187 CD1 PHE 164 1.435 19.093 62.143 1.000 26.16 -615 7 1 1 ANISOU 1187 CD1 PHE 164 2827 3836 3278 135 1188 CD2 PHE ATOM 164 0.414 16.996 62.717 1.000 31.24 ANISOU 1188 CD2 PHE 164 4365 -298 - 96 349 2808 4698 1189 CE1 PHE 164 1.787 18.609 60.894 1.000 30.09 ANISOU 1189 CE1 PHE 164 3609 5052 2771 -148 -1030 641 1190 CE2 PHE 164 0.786 16.501 61.475 1.000 38.25

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- 52 -
                                             -740 -1363 -612
                               4077
                                       3797
ANISOU 1190 CE2 PHE 164 6659
                               17.298 60.588 1.000 32.74
      1191 CZ PHE 164 1.494
                                                   -944 - 385
                   164 3189
                                              712
                               5078
                                       4172
ANISOU 1191 CZ
              PHE
                   165 -2.469 19.609 66.379 1.000 30.62
               PRO
ATOM
       1192 N
                                              -1371 344 -508
               PRO
                               4009
                                       3751
                   165 3876
ANISOU 1192 N
                              19.813 67.809 1.000 33.09
                   165 -2.670
      1193 CA PRO
                                             -190 80 2 3 6
                   165 3299
                                       3510
                               5764
ANISOU 1193 CA PRO
                   165 -1.459
                               19.408 68.638 1.000 36.32
               PRO
       1194 C
MOTA
                    165 3538
                                              664
                                5745
                                       4518
ANISOU 1194 C
               PRO
                    165 -0.776 18.428 68.371 1.000 32.94
       1195 0
               PRO
MOTA
                                              220
                                                    501 387
                                       3487
                                4761
ANISOU 1195 O
               PRO
                    165 4268
                    165 -3.882 18.929 68.123 1.000 38.44
MOTA
       1196 CB
               PRO
                                              -765 271 827
                    165 3807
                               6924
                                       3873
               PRO
ANISOU 1196 CB
                                       66.845 1.000 35.82
                    165 -4.635 18.842
               PRO
       1197 CG
ATOM
                                                688 - 828
                               7020
                                       3995
                                              5
                    165 2595
ANISOU 1197 CG
               PRO
                    165 -3.690 19.130 65.710 1.000 33.90
       1198 CD
               PRO
ATOM
                                             -1149 194 169
                    165 3192
                                       3770
                               5919
ANISOU 1198 CD PRO
                                        68.180 1.000 64.52
                    178 7.727
                               7.453
       1199 N
               LEU
ATOM
                                                    -218 3721
                                        6843 278
                               5376
ANISOU 1199 N
                LEU
                    178 12297
                                        66.973 1.000 43.31
                    178 7.629
                                8.260
       1200 CA
               LEU
MOTA
                                        3168 -984 -2821 -135
                                2730
ANISOU 1200 CA
                    178 10557
               LEU
                                        66.662 1.000 47.36
                               8.539
                    178 6.159
                LEU
MOTA
       1201 C
                                             -2598 -1186 1204
                                3530
                                        5225
                LEU
                    178 9239
ANISOU 1201 C
                                        66.796 1.000 56.53
                                7.659
                     178 5.314
       1202 0
                LEU
ATOM
                                        4076 -4835 1265 -602
                     178 11777
                                5626
ANISOU 1202 O
                LEU
                                        65.746 1.000 55.55
                                7.582
               LEU
                     178 8.222
       1203 CB
ATOM
                                               -1314 -1197 -1822
                     178 11470
                                        5902
               LEU
                                3734
ANISOU 1203 CB
                                        65.774 1.000 62.34
                                7.092
                     178 9.662
       1204 CG
               LEU
MOTA
                                        7760 -1971 194 -443
                                5116
                     178 10812
ANISOU 1204 CG LEU
                                        64.579 1.000 54.23
                     178 9.916
                                6.185
       1205 CD1 LEU
MOTA
                                               1878 -3799 511
                                        5988
ANISOU 1205 CD1 LEU
                     178 9626
                                4989
                                        65.773 1.000 66.44
                                8.264
                     178 10.633
       1206 CD2 LEU
MOTA
                                        10526 -1170 4090 -516
                                3454
ANISOU 1206 CD2 LEU
                     178 11265
                                        66.192 1.000 52.90
                                9.751
       1207 N
                ARG
                     179 5.879
MOTA
                                                     1230 1031
                     179 7853
                                        8421
                                               102
                                3826
ANISOU 1207 N
                ARG
                                        65.807 1.000 51.26
                                10.033
 MOTA
        1208 CA ARG
                     179 4.495
                                               -229 1890 -383
                     179 7235
                                        7421
                                4820
 ANISOU 1208 CA ARG
                                        64.383 1.000 55.25
                                9.563
                     179 4.242
        1209 C
                ARG
 ATOM
                                               -946 2260 -1134
                                6083
                                        7731
                     179 7178
 ANISOU 1209 C
                ARG
                                        64.021 1.000 58.51
                                 9.211
                     179 3.120
        1210 0
                ARG
 MOTA
                                        7565
                                               -1820 3675 -2851
                     179 7036
                                7628
 ANISOU 1210 O
                ARG
                                 11.512 66.040 1.000 41.49
        1211 CB
                     179 4.180
                ARG
 MOTA
                                               -155 1916 1137
                                 4448
                                        4716
 ANISOU 1211 CB
                     179 6600
                ARG
                                 11.700 67.277 1.000 43.15
        1212 CG
                ARG
                     179 3.293
 MOTA
                                        4367
                                               90 1338 530
                                 5908
                     179 6120
 ANISOU 1212 CG
                ARG
                                 12.059 66.833 1.000 47.63
        1213 CD
                     179 1.888
                ARG
 ATOM
                                                     860 -531
                                               195
                                 7453
                                        4463
                      179 6180
 ANISOU 1213 CD
                ARG
                                        67.269 1.000 52.00
                                 13.367
        1214 NE
                      179 1.459
                ARG
 MOTA
                                                     -1168 -538
                                 7834
                                         4539
                                               1669
                      179 7384
 ANISOU 1214 NE
                ARG
                                 14.470 66.556 1.000 64.81
                      179 1.322
        1215 CZ
                ARG
 ATOM
                                                1457 -1107 6 3
                      179 10838
                                 8000
                                         5788
 ANISOU 1215 CZ
                ARG
                                 14.518 65.268 1.000 59.74
        1216 NH1 ARG
                      179 1.637
 ATOM
                                                3628 -2691 445
                                 8090
                                         5074
                      179 9535
 ANISOU 1216 NH1 ARG
                                 15.606 67.117 1.000 65.83
                      179 0.907
        1217 NH2 ARG
 MOTA
                                                4171 -776 1200
                                         5478
 ANISOU 1217 NH2 ARG
                      179 10451
                                 9083
                                         63.589 1.000 43.96
                                 9.501
                 MET
                      180 5.304
        1218 N
 MOTA
                                                     852 -1245
                                         7550
                                                705
                                 3769
                      180 5383
 ANISOU 1218 N
                 MET
                                         62.210 1.000 40.44
                                 9.035
                      180 5.264
        1219 CA MET
  MOTA
                                                -398 574 -1482
                      180 2356
                                 5467
                                         7543
  ANISOU 1219 CA
                 MET
                                         61.920 1.000 43.91
                                  8.258
                 MET
                      180 6.552
         1220 C
  MOTA
                                                18 320 - 2324
                                         7733
                      180 2731
                                  6220
                 MET
  ANISOU 1220 C
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1221 0 MET 180 7.629 8.679 62.327 1.000 39.46 ATOM ANISOU 1221 O 180 2377 5064 -395 906 -912 MET 7554 1222 CB 180 5.129 MET 61.219 1.000 49.84 MOTA 10.189 ANISOU 1222 CB MET 180 2749 7966 8223 -452 -1114 7 2 MOTA 1223 CG MET 180 5.339 9.818 59.757 1.000 62.58 7587 ANISOU 1223 CG 180 7280 8911 MET -2331 -3353 -505 11.015 58.608 1.000 74.24 1224 SD MET 180 4.622 ANISOU 1224 SD MET 180 7480 13510 7216 4918 -262 - 905 MOTA 1225 CE MET 180 4.501 10.037 57.110 1.000 79.59 ANISOU 1225 CE MET 180 6119 20000 4120 -1978 1874 - 912 ALA MOTA 1226 N 181 6.376 7.112 61.275 1.000 37.44 ANISOU 1226 N ALA 181 3523 5646 5055 -271 882 -1132 181 7.407 181 3980 1227 CA MOTA ALA6.140 60.986 1.000 37.40 ANISOU 1227 CA 3980 ALA 6250 -625 2048 4 6 1 1228 C ALA 181 8.287 6.591 ATOM 59.837 1.000 31.49 ANISOU 1228 C ALA 181 2975 3842 5149 -32 920 181 7.834 1229 0 ALA 7.393 58.997 1.000 30.77 MOTA 181 2903 ANISOU 1229 O ALA 4765 4021 197 -98 164 ALA MOTA 1230 CB 181 6.727 4.817 60.620 1.000 42.66 ANISOU 1230 CB ALA 181 4105 4284 7820 -1023 1629 5 5 7 1231 N 182 9.541 ATOM PRO 6.137 59.840 1.000 24.52 4237 ANISOU 1231 N PRO 182 2782 2296 -240 -76 320 1232 CA PRO 182 10.442 6.667 58.820 1.000 20.55 ATOM ANISOU 1232 CA PRO 182 2612 2870 2326 -335 -117 - 65 ATOM 1233 C PRO 182 9.958 6.402 57.408 1.000 19.31 ANISOU 1233 C 182 2609 PRO 2491 -391 48 - 86 2236 MOTA 1234 0 PRO 182 9.448 5.326 57.080 1.000 21.68 ANISOU 1234 O PRO 182 2991 2759 -440 -340 - 55 2486 182 11.768 5.939 1235 CB PRO ATOM 59.047 1.000 24.98 ANISOU 1235 CB PRO 182 2589 3860 3042 -170 -286 1 5 3 60.393 1.000 28.42 ATOM 1236 CG PRO 182 11.681 5.351 ANISOU 1236 CG 182 3352 PRO 3582 3863 656 321 1038 182 10.215 5.210 MOTA 1237 CD PRO 60.747 1.000 32.21 ANISOU 1237 CD PRO 182 3333 -826 -390 1785 4905 4000 183 10.111 7.414 56.561 1.000 19.27 1238 N ATOM HIS ANISOU 1238 N HIS 183 2131 -274 -204 1 7 6 2658 2533 1239 CA HIS 55.144 1.000 18.01 ATOM 183 9.757 7.306 ANISOU 1239 CA HIS 183 1882 2311 2652 -341 -455 3 4 6 ATOM 1240 C HIS 183 10.749 8.124 54.337 1.000 15.74 ANISOU 1240 C HIS 183 1964 1560 2456 -75 -352 1 2 8 1241 0 MOTA HIS 183 11.355 9.061 54.868 1.000 18.14 ANISOU 1241 O HIS 183 2297 2093 2504 -509 -127 -135 54.835 1.000 18.66 1242 CB HIS 7.781 ATOM 183 8.338 -136 -243 3 7 1 ANISOU 1242 CB HIS 183 1970 2173 2945 MOTA 1243 CG HIS 183 8.089 9.120 55.447 1.000 26.67 183 3100 183 7.884 ANISOU 1243 CG HIS 2751 4281 262 222 - 306 1244 ND1 HIS 56.800 1.000 35.36 9.362 ANISOU 1244 ND1 HIS 183 4432 4078 4926 -1190 1466 -1454 10.311 54.821 1.000 33.00 1245 CD2 HIS MOTA 183 8.051 1687 -677 -173 ANISOU 1245 CD2 HIS 183 4117 2522 5898 1246 CE1 HIS 183 7.739 ATOM 10.658 56.980 1.000 35.91 ANISOU 1246 CE1 HIS 183 2611 -472 -625 -2616 6565 4468 1247 NE2 HIS 183 7.829 ATOM 11.251 55.798 1.000 40.55 ANISOU 1247 NE2 HIS 1821 -1013 -1590 183 4375 3417 7614 MOTA 1248 N TYR 184 10.890 7.778 53.061 1.000 15.68 ANISOU 1248 N -124 -470 1 0 7 TYR 184 1973 1551 2434 1249 CA TYR MOTA 184 11.605 8.685 52.152 1.000 14.81 ANISOU 1249 CA TYR -312 1 4 5 184 1798 1392 2438 147 1250 C ATOM TYR 184 10.572 9.239 51.169 1.000 14.53 ANISOU 1250 C TYR 184 1656 2416 -70 -399 9 8 1449 MOTA 1251 0 TYR 184 9.468 8.728 51.045 1.000 15.83

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ATOM 1282 N MET ANISOU 1283 CA MET ANISOU 1283 CA MET ANISOU 1284 C MET ANISOU 1285 O MET ANISOU 1285 O MET ANISOU 1286 CB MET ANISOU 1286 CB MET ANISOU 1287 CG MET ANISOU 1288 SD MET ANISOU 1288 SD MET ANISOU 1288 SD MET ANISOU 1288 SD MET ANISOU 1289 CE MET ANISOU 1289 CE MET ANISOU 1290 N VAL ANISOU 1290 N VAL ANISOU 1291 CA VAL ANISOU 1291 CA VAL ANISOU 1292 C VAL ANISOU 1292 C VAL ANISOU 1293 O VAL ANISOU 1293 O VAL ANISOU 1294 CB VAL ANISOU 1295 CG1 VAL ANISOU 1295 CG1 VAL ANISOU 1295 CG1 VAL ANISOU 1296 CG2 VAL ANISOU 1296 CG2 VAL ANISOU 1296 CG2 VAL ANISOU 1297 N THR ANISOU 1297 N THR ANISOU 1298 CA THR ANISOU 1299 C THR ANISOU 1300 O THR ANISOU 1300 CB THR ANISOU 1301 CB THR ANISOU 1301 CB THR ANISOU 1302 CG1 THR ANISOU 1302 CG1 THR ANISOU 1302 CG2 THR ANISOU 1303 CG2 THR ANISOU 1304 N LEU ANISOU 1304	188 10.898 14.844 43.292 1.000 13.44 188 1552 1334 2221 -64 -34 -26 188 12.215 15.380 42.878 1.000 12.11 188 1508 1261 1833 29 -60 -61 188 12.853 16.022 44.104 1.000 12.78 188 1563 1156 2136 167 -311 - 42 188 1408 1390 2294 116 -264 -26 188 12.038 16.300 41.667 1.000 13.40 188 1408 1390 2294 116 -264 -2 6 188 1565 1501 2123 44 -161 20 7 188 13.296 17.095 41.315 1.000 13.66 188 1565 1501 2123 44 -161 20 7 188 13.296 17.095 41.315 1.000 14.05 188 1697 1595 2046 66 150 133 188 14.600 15.971 40.752 1.000 14.05 188 16565 1591 2529 109 -81 1 1 0 188 16.005 17.102 40.686 1.000 17.74 188 1852 2032 2855 -242 505 1 2 1 189 12565 17.671 44.616 1.000 12.62 189 1586 1203 2007 103 -147 -134 189 12.565 17.671 45.918 1.000 12.60 189 1412 1438 1937 -228 -11 - 4 4 189 11.285 17.968 46.679 1.000 12.56 189 1446 1291 2036 21 -320 - 4 9 189 13.440 18.955 45.856 1.000 12.95 189 13.440 18.955 45.856 1.000 15.56 189 1376 2094 2437 -140 161 9 1 189 12.730 20.056 45.082 1.000 15.00 189 1763 1391 2547 -130 -483 8 1 190 11.425 18.067 47.984 1.000 12.47 190 10.353 18.454 48.897 1.000 15.00 189 1763 1391 2547 -130 -483 8 1 190 11.425 18.067 47.984 1.000 12.47 190 10.879 19.630 49.710 1.000 12.47 190 10.879 19.630 49.710 1.000 12.47 190 1178 1436 2124 -32 -297 -23 2 190 11.959 19.523 50.320 1.000 15.06 190 1424 1767 2531 46 -571 -446 190 9.913 17.297 49.808 1.000 12.47 190 1693 1469 1386 -168 80 -121 190 10.879 19.630 49.710 1.000 12.47 190 1693 1469 1386 -168 80 -121 190 10.879 19.630 49.710 1.000 12.47 190 1693 1469 2334 -100 -25 -194 190 19.8778 17.723 50.734 1.000 14.79 190 1693 1469 2334 -100 -25 -194 190 10.148 20.724 49.732 1.000 12.97 191 1329 1449 23 -21 -286 1000 12.75 191 10.148 20.724 49.732 1.000 12.97 191 10.148 20.724 49.732 1.000 12.97 191 10.148 20.724 49.732 1.000 12.97 191 10.148 20.724 49.732 1.000 12.97 191 10.148 20.724 49.732 1.000 12.97 191 10.148 20.724 49.732 1.000 12.97 191 10.148 20.724 49.732 1.000 12.97 191 10.148 20.724 49.732 1.000 12.97 191 10.148 20.724 49.732 1.000 12.97 191 10.148 20.724 49.732 1.000 12.97
ANISOU 1298 CA THR ATOM 1299 C THR ANISOU 1299 C THR ATOM 1300 O THR ANISOU 1300 O THR ATOM 1301 CB THR ANISOU 1301 CB THR ANISOU 1301 CB THR ANISOU 1302 OG1 THR ANISOU 1302 OG1 THR ANISOU 1303 CG2 THR	190 1292 1356 1903 -57 -221 -151 190 10.879 19.630 49.710 1.000 12.47 190 1178 1436 2124 -32 -297 -232 190 11.959 19.523 50.320 1.000 15.06 190 1424 1767 2531 46 -571 -446 190 9.913 17.297 49.808 1.000 13.16 190 1509 1605 1886 -168 80 -121 190 9.481 16.201 48.993 1.000 14.47 190 1693 1469 2334 -100 -25 -194 190 8.778 17.723 50.734 1.000 14.79
ATOM 1304 N LEU	191 10.148 20.724 49.732 1.000 12.97
ANISOU 1311 CD2 LEU ATOM 1312 N ILE	191 2297 1906 2837 -345 -437 1 4 8 192 10.199 22.148 52.946 1.000 15.36

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						- 56 -			
ANISOU	1312	N	ILE	192	1479	2152	2204	-47	-165 - 164
ATOM	1313		ILE		9.417	22.162			
ANISOU			ILE			22.102	54.194		
					1456	2043	2251		
ATOM	1314		ILE	192	9.692	23.423	55.010	1.000	15.58
ANISOU	1314	С	ILE	192	1696	1973	2251	-199	
ATOM	1315	0	ILE		10.836				
ANISOU				100	10.030	23.691	55.381	1.000	17.20
			ILE		1856	2449	2229	-307	-341 - 574
ATOM	1316		ILE	192	9.722	20.920	55.040	1 000	17 03
ANISOU	1316	CB	ILE		2246	1958	2266	-52	325 - 303
MOTA	1317				9.454	19.596			345 - 303
ANISOU							54.317	1.000	
					3040	2010	2473		128 - 382
MOTA	1318	CG2	ILE	192	8.995	20.967	56.403	1.000	18 14
ANISOU	1318	CG2	ILE	192	2278	2354	2262	229	290 - 258
ATOM	1319				9.420			1 000	230 - 238
ANISOU	1310	CD1	Tre				55.235		
					4658	2114	5222	-398	
ATOM	1320		GLN		8.625	24.172	55.249	1.000	17.04
ANISOU	1320	N	${ t GLN}$	193	2042	2185	2248	112	-388 - 301
ATOM	1321	CA	GLN		8.680	25.291	56.201	1 000	
ANISOU			GLN		1737		30.201		
ATOM	1322					2167	2824		
			GLN		7.898	24.869	57.443	1.000	19.67
ANISOU			${ t GLN}$	193	1882	2624	2969	-232	211 -840
ATOM	1323	0	GLN	193	7.082	23.942	57.426	1 000	25 60
ANISOU	1323	<u> </u>	GLN		2066		37.420		
ATOM	1324					3843	4197		-110 6 2
-			GLN		8.129	26.598	55.643	1.000	23.74
ANISOU			${ t GLN}$	193	3070	2388	3561	500	-98 -514
\mathtt{ATOM}	1325	CG	${ t GLN}$	193	8.913		54.559		
ANISOU	1325	CG	GLN		4664		3600		
ATOM	1326		GLN				3689	656	209 0
					8.338	28.665	54.156		26.30
ANISOU			GLN		2868	2943	4181	791	3 1 1 1
\mathtt{ATOM}	1327	OE1	GLN	193	7.193	28.695	53.688		
ANISOU	1327	OE1	GLN	193	2826	7147	7241	-51	
ATOM	1328	MES	CIN		9.080				-616 3173
ANISOU	1220	NTTO	GLM			29.748	54.345		
AMISOU	1320	NEZ			3609	2588	5368	418	1259 6 9 2
ATOM	1329		GLN		8.241	25.259	58.645	1.000	22.04
ANISOU	1329	N	GLN	194	2926	2758	2690	303	-368 - 83
ATOM	1330	CA	GLN		7.569	24.793			
ANISOU			GLN				59.847		
ATOM	1331				3144	2617	2855	82 -23	30 -150
			GLN		7.275	26.054	60.663	1.000	22.19
ANISOU	1331	C	${ t GLN}$	194	2809	2768	2856	117	- 396 - 320
MOTA	1332	0	GLN	194	7.889	27.100	60.418		
ANISOU	1332	\cap	GLN		4041				
ATOM	1333						2679		
			GLN		8.467	23.943	60.739	1.000	29.21
ANISOU			GLN	194	4493	2707	3899	477	-50 939
\mathtt{ATOM}	1334		${ t GLN}$	194	9.105	22.735	60.083		
ANISOU	1334	CG	GLN		3108	3530	4305	576	
ATOM	1335		GLN						-121 4 9 4
ANISOU	1225	C.T.		124	10.296	22.332	60.962		
			GLN		2961	5384	3800	824	359 1075
ATOM	1336	OE1	GLN	194	11.421		60.474		27 28
ANISOU	1336	OE1	GLN		2781	4189	3397		
ATOM	1337	MES	CIN					118	133 - 249
	1227	3700	GTM		9.998	22.100	62.232		
ANISOU					3540	3958	3832	989	645 800
ATOM	1338	N	THR	195	6.419	25.891	61.658		
ANISOU	1338	N	THR		2407	3058	3387	-211	
ATOM	1339		THR		6.476				
ANISOU						26.833	62.768		
			THR		3459	3544	3308		0 - 8 9 0
ATOM	1340		THR		6.933	25.997	63.958		
ANISOU			THR	195	3825	2829	3268	558	19 -1247
MOTA	1341	0	THR		6.639		63.994		10 17
ANISOU			THR		2973				
ATOM	1342					2916	4815	481	171 -1030
			THR		5.149	27.534	63.069	1.000	25.87
	+ 4 /1 - 3	CB	THR	195	3428	2849	3551	-16	
ANISOU	1247					4043	J J J L	T O	-592 -1137

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						- 57 -				
ATOM	1343	OG1	THR	195 4	4.111	26.550	63.196	1.000	25.45	
ANISOU	1343	OG1	THR	195	3427	3101			7 - 750	
ATOM	1344	CG2	THR	195	4.788	28.396	61.847			
ANISOU				195		2552	4380		-70 -409	
ATOM	1345		PRO		7.604	26.587	64.923			
ANISOU			PRO	196		3191			-517 -1542	
ATOM	1346		PRO		8.101	25.823	66.065			
ANISOU			PRO		3113	3700			-441 - 646	
ATOM	1347		PRO		7.018	25.534				
							67.096			
ANISOU			PRO	196		3326			-1381	
ATOM	1348		PRO		6.002	26.229	67.192			
ANISOU			PRO		4146	4649			-180 -1658	
MOTA	1349		PRO		9.094	26.816	66.694			
ANISOU			PRO		3888	3292	4111		-353 -1072	
ATOM	1350		PRO		8.533	28.174				
ANISOU			PRO		6285	3575	3390		-1326 -133	3 2
ATOM	1351		PRO		7.897	28.035	65.012			
ANISOU			PRO		6407	3606	2600		-494 -1031	
ATOM	1352		CYS		7.289	24.533	67.919	1.000	26.96	
ANISOU			CYS		2739	4038	3465	-113	85 -1227	
MOTA	1353		CYS	197	6.519 3979	24.289	69.126	1.000	31.73	
ANISOU	1353	CA	CYS	197	3979	4543	3533	-39	721 -1726	1
ATOM	1354	C	CYS	197	6.803		70.124	1.000	35.58	
ANISOU	1354	С	CYS		4213	4819	4486	-480	1126 - 2282	:
ATOM	1355	0	CYS		7.917	25.939	70.175			
ANISOU	1355	0	CYS		3817	4845	3246			
ATOM	1356		CYS		6.940	22.962	69.767	1.000		
ANISOU			CYS		5913	4705	2980		1566 - 1423	}
MOTA	1357		CYS		6.553		68.741			
ANISOU			CYS		3605	4224	3009			
ATOM	1358		ALA				70.866			
ANISOU			ALA	198	5.771 5038 5.983	4984	4139		1647 - 2070)
ATOM	1359		ALA	198	5.983	26.811	71.888			
ANISOU			ALA		6273	4144	3230		522 -1230)
MOTA	1360		ALA		6.993	26.328	72.921			
ANISOU			ALA		5998	6138				
ATOM	1361		ALA		7.759	27.127				
ANISOU			ALA		5209	6328	4742) - 5 5 5	
ATOM	1362		ALA		4.671	27.231	72.532			
ANISOU			ALA		7588	5697			1068 - 721	
ATOM	1363		ASN		7.036	25.036				
ANISOU			ASN		4027		3270	805	167 - 621	
ATOM	1364				7.969	24 578	74.264	1 000		
ANISOU			ASN		3643	6167	2950	-670	-265 - 808	
ATOM	1365		ASN		9.352	24.262			31.53	
ANISOU			ASN		4077	5048	2853	384	-420 - 855	
ATOM	1366		ASN		10.153				36.33	
ANISOU			ASN			23.667	3957	-403	-1305 -12	6
ATOM	1367		ASN		4223	5624 23.308			36.38	Ü
ANISOU					7.441					
			ASN		4533	5029	4262	859	584 - 522	
ATOM	1368		ASN		7.198	22.180			31.28 202 178	
ANISOU			ASN		4030	4863	2993	882		
ATOM			ASN		7.743	22.151			37.62	
ANISOU					4693	6272	3330	122	728 - 56	
ATOM			ASN		6.393	21.190			36.42	
ANISOU					3508	6251	4078	-13	1132 - 958	
ATOM	1371		GLY		9.616	24.569			30.93	
ANISOU			GLY		4342	4232	3179		144 -692	
ATOM	1372		GLY		10.920	24.304			35.26	_
ANISOU			GLY		4430	4905	4060			O
ATOM	1373	C	GLY	200	11.184	22.886	71.429	1.000	36.83	

ANTSOU 1374 O GLY 200 4683				- 58 -		
ATOM 1374 O GLY 200 12.257			00 4683	4375	4936	-360 1601 -1460
ATOM 1375 N PHE 201 10.264 21.638 71.588 1.000 22.666 378 ANISOU 1375 N PHE 201 10.491 20.575 71.106 1.000 27.55 32 ATOM 1376 CA PHE 201 10.491 20.575 71.106 1.000 27.55 32 ATOM 1376 CA PHE 201 10.491 20.575 71.106 1.000 27.55 72 ATOM 1377 C PHE 201 10.752 20.553 69.600 1.000 24.89 ANISOU 1378 O PHE 201 9.994 21.255 68.910 1.000 28.22 ANISOU 1378 O PHE 201 9.994 21.255 68.910 1.000 28.22 ANISOU 1378 O PHE 201 9.994 21.255 68.910 1.000 28.22 ANISOU 1378 O PHE 201 9.994 21.255 68.910 1.000 28.22 ANISOU 1379 CB PHE 201 9.250 19.729 71.413 1.000 30.46 ANISOU 1379 CB PHE 201 9.250 19.729 71.413 1.000 30.46 ANISOU 1380 CB PHE 201 9.425 18.262 71.027 1.000 34.89 ANISOU 1381 CD1 PHE 201 9.425 18.262 71.027 1.000 34.89 ANISOU 1381 CD1 PHE 201 3436 4103 4310 87.72 162 89 ANISOU 1382 CD2 PHE 201 4015 4609 4632 -772 162 89 ANISOU 1382 CD2 PHE 201 2979 4019 3960 329 612 -10.7 ANISOU 1383 CS1 PHE 201 10.564 16.160 71.0078 1.000 28.84 ANISOU 1383 CS1 PHE 201 6489 3608 4239 -1078 -1475 -50.0 ANISOU 1384 CS2 PHE 201 40.761 16.363 69.799 1.000 31.78 ANISOU 1384 CS2 PHE 201 40.761 16.363 69.799 1.000 31.78 ANISOU 1384 CS2 PHE 201 40.761 16.363 69.799 1.000 31.78 ANISOU 1384 CS2 PHE 201 40.761 16.363 69.799 1.000 31.78 ANISOU 1386 C AVAL 202 11.706 19.755 18.606 70.265 10.000 29.78 ANISOU 1386 C AVAL 202 11.706 19.755 18.606 70.265 10.000 29.778 ANISOU 1386 C AVAL 202 11.706 19.755 18.606 70.766 1.000 20.578 ANISOU 1388 C VAL 202 11.706 19.755 18.606 70.766 1.000 29.778 ANISOU 1387 CA VAL 202 11.706 19.755 18.606 70.766 1.000 29.778 ANISOU 1387 CA VAL 202 11.706 19.755 18.606 70.766 1.000 29.778 ANISOU 1388 C VAL 202 11.706 19.755 18.606 70.766 1.000 20.577 ANISOU 1389 O VAL 202 11.706 19.755 18.606 70.766 1.000 20.777 ANISOU 1389 O VAL 202 11.706 19.755 18.606 70.766 1.000 20.777 ANISOU 1389 O VAL 202 11.706 19.755 18.606 70.766 1.000 20.779 ANISOU 1389 O VAL 202 11.706 19.755 18.606 70.706 1.000 20.779 ANISOU 1399 O CER 203 10.168 19.751 19.755 18.606 70.706 1.000 20.779 ANISOU 1399 O CER 203 10.168 19.755 18.606 70.706 1.000 20		_		22.566		
ANISOU 1375 N PHE 201 3813 4229 2847 145 463 -326 ATOM 1376 CA PHE 201 10.491 20.575 71.106 1.000 27.55 ANISOU 1376 CA PHE 201 3190 4337 2943 -233 219 -672 ANISOU 1377 C PHE 201 10.752 20.553 69.600 1.000 24.89 ANISOU 1378 C PHE 201 3583 3184 3977 10 -268 -379 ANISOU 1378 C PHE 201 3583 3184 3977 10 -2421 277 ATOM 1378 O PHE 201 3583 3184 3977 10 -421 277 ATOM 1380 CG PHE 201 3153 4862 366 -371 -40 -73 ANISOU 1380 CG PHE 201 4015 4609 4632 -772 1628 9 ANISOU 1380 CG PHE 201 4015 4609 4632 -772 1628 9 ATOM 1381 CD1 PHE 201 10.395 17.472 71.605 1.000 31.18 ANISOU 1382 CD2 PHE 201 8.613 17.681 70.078 1.000 28.84 ANISOU 1382 CD2 PHE 201 8.613 17.681 70.078 1.000 28.84 ANISOU 1383 CD1 PHE 201 10.564 16.160 71.240 1.000 37.73 ANISOU 1383 CD1 PHE 201 10.564 16.160 71.240 1.000 37.73 ANISOU 1383 CD1 PHE 201 10.564 16.160 71.240 1.000 37.73 ANISOU 1383 CD1 PHE 201 4027 4019 4019 4019 4019 4019 4019 4019 4019						
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ANISOU 1377 C PHE 201 2943 3622 2832 100 288 379 ATOM 1378 O PHE 201 9.994 318.5 68.910 1.000 28.22 7 ATOM 1378 O PHE 201 9.994 318.5 68.910 1.000 28.22 7 ATOM 1378 O PHE 201 9.580 19.729 71.413 1.000 30.46 ANISOU 1379 CB PHE 201 9.25 18.262 71.027 1.000 34.89 ATOM 1380 CG PHE 201 9.425 18.262 71.027 1.000 34.89 ATOM 1381 CD1 PHE 201 10.395 17.472 71.605 1.000 31.18 ANISOU 1381 CD1 PHE 201 10.395 17.472 71.605 1.000 31.18 ANISOU 1382 CD2 PHE 201 3436 4103 4310 -875 -93 -1105 ATOM 1382 CD2 PHE 201 8.613 17.681 70.078 1.000 28.84 ANISOU 1382 CD2 PHE 201 8.613 4609 4632 -772 162 8 9 ATOM 1382 CD2 PHE 201 8.613 4609 4632 -772 162 8 9 ATOM 1382 CD2 PHE 201 8.613 4609 4632 -772 162 8 9 ATOM 1382 CD2 PHE 201 8.613 4609 4632 -772 162 8 9 ATOM 1382 CD2 PHE 201 8.613 470 4019 3960 329 612 -107 ATOM 1382 CD2 PHE 201 8.613 4609 4632 -772 1605 1.000 37.73 ANISOU 1382 CD2 PHE 201 8.613 4609 4019 3960 329 612 -107 ATOM 1383 CE1 PHE 201 10.564 16.363 69.679 1.000 37.73 ANISOU 1383 CE1 PHE 201 4327 3911 3838 652 250 119 ATOM 1384 CE2 PHE 201 3705 3397 4211 6 -638 -849 ATOM 1386 V VAL 202 211.706 19.755 40.000 29.78 ANISOU 1386 C VAL 202 11.969 19.626 67.706 1.000 22.75 ANISOU 1387 CA VAL 202 11.969 19.626 67.706 1.000 22.75 ANISOU 1388 C VAL 202 11.969 19.626 67.706 1.000 22.75 ANISOU 1388 C VAL 202 11.880 17.190 67.541 1.000 22.75 ANISOU 1389 C VAL 202 2729 348 257 67.198 1.000 22.75 ANISOU 1389 C VAL 202 2729 348 257 67.198 1.000 22.75 ANISOU 1389 C VAL 202 2826 3868 3887 -490 474 -39 ANISOU 1390 CB VAL 202 13.476 19.721 67.823 1.000 24.99 ANISOU 1390 CB VAL 202 13.476 19.721 67.823 1.000 27.70 ANISOU 1390 CB VAL 202 13.476 19.721 67.823 1.000 27.70 ANISOU 1390 CB VAL 202 13.476 19.721 67.823 1.000 24.99 ANISOU 1390 CB VAL 202 13.476 19.721 67.823 1.000 24.99 ANISOU 1390 CB VAL 202 13.476 19.721 67.823 1.000 27.70 ANISOU 1390 CB VAL 202 13.750 19.464 65.393 1.000 27.70 ANISOU 1390 CB VAL 202 13.750 19.751 67.823 1.000 27.70 ANISOU 1390 CB VAL 202 13.753 19.464 65.933 1.000 27.70 ANISOU 1390 CB VAL 202 13.753 19.464 66.331 1.0						
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ANISOU 1393 N SER 203 2194 3607 3356 -31 -179 -528 ATOM 1394 CA SER 203 9.634 17.231 65.940 1.000 23.70 ANISOU 1394 CA SER 203 2373 3584 3046 -290 308 -533 ATOM 1395 C SER 203 10.168 16.511 64.710 1.000 21.28 ANISOU 1395 C SER 203 2173 3041 2871 46 227 - 42 ATOM 1396 O SER 203 10.159 15.285 64.640 1.000 27.60 ANISOU 1396 O SER 203 4105 3097 3284 -482 1010 - 249 ATOM 1397 CB SER 203 8.148 17.571 65.685 1.000 29.06 ANISOU 1397 CB SER 203 2251 3790 5001 -180 203 -2064 ATOM 1398 OG SER 203 7.584 18.175 66.843 1.000 32.55 ANISOU 1398 OG SER 203 3840 4298 4231 920 1099 -382 ATOM 1399 N LEU 204 10.688 17.233 63.724 1.000 22.46 ANISOU 1399 N LEU 204 2476 3013 3043 79 450 - 46 ATOM 1400 CA LEU 204 11.166 16.530 62.544 1.000 20.26 ANISOU 1400 CA LEU 204 12.595 16.038 62.747 1.000 18.83 ANISOU 1401 C LEU 204 2151 2528 2477 -75 60 - 1 ATOM 1402 O LEU 204 2333 2386 3059 -303 -195 4 0 4 ATOM 1403 CB LEU 204 13.443 16.783 63.251 1.000 20.47 ANISOU 1402 O LEU 204 2333 2386 3059 -303 -195 4 0 4 ATOM 1403 CB LEU 204 11.103 17.486 61.362 1.000 21.42						
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ATOM 1402 O LEU 204 13.443 16.783 63.251 1.000 20.47 ANISOU 1402 O LEU 204 2333 2386 3059 -303 -195 4 0 4 ATOM 1403 CB LEU 204 11.103 17.486 61.362 1.000 21.42						
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ANISOU 1403 CB LEU 204 2718 2548 2871 311 -16 - 8	ANISOU 1403					

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				- 39 -		
ATOM	1404 CG	1.711	204 9.769	18.188	61 070	1 000 21 57
						1.000 33.57
	1404 CG		204 2820	4319		
ATOM	1405 CI	01 LEU	204 9.797	18.747	59.660	1.000 36.19
ANTSOU	1405 CI	1 LEII	204 4402	3807	5540	
ATOM						
	1406 CI		204 8.581	17.234	61.219	1.000 37.76
ANISOU	1406 CI)2 LEU	204 3058	5328	5960	-526 -1896 686
ATOM	1407 N	${ t GLN}$	205 12.864			1.000 20.33
	1407 N				02.204	
		GLN	205 2518	2644	2563	104 -31 -129
ATOM	1408 CA	A GLN	205 14.209	14.247	62.335	1.000 18.88
ANISOU	1408 CA	A GLN	205 2522	2225		
ATOM	1409 C				2425	-6 -181 3 6
		${ t GLN}$	205 14.512	13.504	61.036	1.000 18.19
ANISOU	1409 C	${ t GLN}$	205 1986	2383	2543	-143 -188 - 80
ATOM	1410 0	GLN	205 13.577	13.033		1.000 19.87
	1410 0				00.400	
		GLN	205 1974	3063	2514	-125 -212 -237
ATOM	1411 CE	3 GLN	205 14.296	13.267	63.493	1.000 24.25
ANISOU	1411 CE	GLN	205 3948	2716	2548	202 -343 2 9 6
ATOM	1412 CG		205 14.164			
_						1.000 30.64
ANISOU	1412 CG		205 4099	5159	2382	850 -327 - 8 9
\mathtt{ATOM}	1413 CI	GLN	205 14.744	13.078		1.000 28.28
ANTSOIL	1413 CI		205 4473			
				3633	2640	
MOTA	1414 OF		205 14.307	11.921	66.041	1.000 37.69
ANISOU	1414 OE	El GLN	205 5733	5073	3515	-2145 -699 4 7 8
ATOM	1415 NE	2 GLM	205 15.710			
	1415 NE	CTN				1.000 40.53
			205 6798	4417		-1341 -2865 323
\mathtt{ATOM}	1416 N	ALA	206 15.752	13.471	60.576	1.000 18.52
ANISOU	1416 N	ALA	206 2070	2199	2769	
ATOM	1417 CA					
			206 16.152	12.700	59.405	1.000 18.42
	1417 CA	ALA	206 2074	2351	2575	-100 -158 2 3
\mathtt{ATOM}	1418 C	ALA	206 17.343	11.802		1.000 17.41
ANTSOU	1418 C	ALA	206 2107			
				2158	2350	
ATOM	1419 0	ALA	206 18.123	12.203	60.613	1.000 20.67
ANISOU	1419 0	ALA	206 2469	2410	2973	
ATOM	1420 CE	3 ALA	206 16.637	13.599		1.000 18.77
ANISOU			206 20:03,			
			206 2119	2310	2703	156 -65 147
ATOM	1421 N	GLU	207 17.492	10.764	58.931	1.000 18.09
ANISOU	1421 N	GLU	207 2092	2101	2680	-249 -496 -162
MOTA	1422 CA		207 18.710	9.944		
	1422 CA					1.000 19.48
			207 2210	2091	3100	-73 -432 - 44
ATOM	1423 C	${ t GLU}$	207 19.851	10.730	58 320	1.000 19.98
ANISOU	1423 C	GLU	207 2018	2233	3342	220 -560 5 4 4
ATOM	1424 0					
		GLU	207 19.732	11.068	57.143	1.000 20.33
	_	GLU	207 2000	2753	2970	5 -471 8 9
\mathtt{ATOM}	1425 CE	GLU	207 18.566	8.623		1.000 24.03
ANTSOU	1425 CE	CT.II	207 3401	1784		
ATOM					3946	316 -1226 6 1
	1426 CG		207 19.757	7.674	58.295	1.000 24.35
ANISOU	1426 CG	GLU	207 3223	1907	4121	354 93 4 6 7
ATOM	1427 CI	GLU	207 20.730	7.791		
	1427 CI					1.000 31.69
			207 2729	5178	4134	-1218 -175 1 2 2
\mathtt{ATOM}	1428 OF	El GLU	207 20.376	7.611	55.943	1.000 26.97
ANISOU	1428 OF	El GLU	207 2849	3404	3993	
ATOM	1429 OF					
	1400 C	12 GTO	207 21.908	8.121		1.000 30.70
	1429 OE		207 2484	3416	5764	- 233 <i>-</i> 342 <i>-</i> 1168
\mathtt{ATOM}	1430 N	VAL	208 20.919	10.936		1.000 18.53
ANISOU	1430 N	VAL	208 2020			
ATOM				2112	2907	130 -362 3 2 0
	1431 CA		208 22.150		58.541	1.000 19.53
ANISOU	1431 CA	VAL	208 2044	2238	3137	39 -476 630
ATOM	1432 C	VAL	208 23.341	10.755		1.000 21.95
	1432 C	VAL	208 2040			
ATOM				2792	3507	225 -461 7 9 7
	1433 0	VAL	208 23.460	10.663	60.314	1.000 23.82
	1433 0	VAL	208 2262		3547	
ATOM	1434 CE	3 VAL	208 22.271	13 027	58 905	1.000 19.72
			<u></u>	17.04/	20.203	1.000 17.72

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ANISOU 1434 CB VAL 208 1918 2429 3145 -47 -308 3 ATOM 1435 CG1 VAL 208 23.524 13.626 58.281 1.000 23.14 -308 3 1 1 ANISOU 1435 CG1 VAL 208 2524 3895 2374 -202 284 349 1436 CG2 VAL 208 21.030 13.812 58.469 1.000 19.47 ANISOU 1436 CG2 VAL 208 2462 2279 2658 -667 - 87 232 208 2462 2279 2658 232 -667 -209 24.180 10.169 58.246 1.000 23.88 209 2500 2449 4123 465 -711 3 209 25.306 9.374 58.773 1.000 26.42 209 1987 3599 4450 460 -487 5 209 24.905 8.250 59.695 1.000 30.01 1437 N ATOM $\operatorname{\mathsf{GLY}}$ ANISOU 1437 N GLY-711 3 6 1438 CA GLY ANISOU 1438 CA GLY -487 5 1 6 ATOM 1439 C GLY ANISOU 1439 C 209 3469 4693 GLY 3240 238 -1422 209 25.609 7.835 60.629 1.000 31.45 209 4053 4458 3438 1225 -897 8 1440 0 ATOM GLY ANISOU 1440 O GLY 1225 -897 8 3 1441 N ATOM GLY 210 23.691 7.702 59.523 1.000 26.64 ANISOU 1441 N GLY 210 3165 3214 3744 259 -86 350 210 23.263 6.585 60.360 1.000 29.78 210 4603 3091 3619 -55 -997 5 8 4 1442 CA GLY MOTA ANISOU 1442 CA GLY 210 4603 3091 3619 -55 -997 5 8 4

ATOM 1443 C GLY 210 22.622 6.993 61.663 1.000 38.28

ANISOU 1444 C GLY 210 5827 4212 4507 -2536 732 5 0

ATOM 1444 O GLY 210 22.160 6.187 62.481 1.000 41.45

ANISOU 1444 O GLY 210 4152 6516 5082 -1874 -567 2 3 4 6

ATOM 1445 N ALA 211 22.512 8.274 61.976 1.000 32.81

ANISOU 1445 N ALA 211 4803 4625 3037 1372 -1177 6 3 2

ATOM 1446 CA ALA 211 21.828 8.603 63.235 1.000 35.62

ANISOU 1446 CA ALA 211 3993 5958 3584 1061 -610 9 7 0

ATOM 1447 C ALA 211 3508 4737 3699 302 69 1854

ATOM 1448 O ALA 211 3508 4737 3699 302 69 1854

ATOM 1448 O ALA 211 3661 4062 3020 -571 -551 1010

ATOM 1449 CB ALA 211 3661 4062 3020 -571 -551 1010

ATOM 1449 CB ALA 211 3644 8904 3169 1372 -18 -7 9 1

ATOM 1450 N PHE 212 19.682 9.676 63.825 1.000 36.68

ANISOU 1450 N PHE 212 5211 4237 4489 1166 1265 217 1

ATOM 1451 CA PHE 212 18.620 10.654 63.641 1.000 28.82

ANISOU 1451 CA PHE 212 4490 3167 3293 263 504 10 3 7 ANISOU 1442 CA GLY 210 4603 ANISOU 1451 CA PHE 212 4490 212 4490 3167 3293 263 504 1037 212 19.100 12.023 64.124 1.000 34.72 MOTA 1452 C PHEANISOU 1452 C PHE 212 6746 3760 2685 -248 -539 7 7 6 ATOM 1453 0 PHE 212 19.667 12.191 65.210 1.000 39.12 ANISOU 1453 O 212 6144 PHE 5384 3335 -549 -1129 1220 2569 8288 1348 3748 2314 662 -581 1 0 0 -810 - 323-855 - 643 -328 -580 -179 189 -356 - 798 -410 5 2 0 1461 CG2 THR 213 20.735 16.254 62.355 1.000 29.45 ANISOU 1461 CG2 THR 213 4422 3320 3448 -106 -1265 214 18.119 16.177 64.371 1.000 21.05 214 2790 2236 2972 -82 -380 -ATOM 1462 N ASP ANISOU 1462 N ASP 214 2790 -380 - 1421463 CA ASP 214 17.001 17.110 64.462 1.000 20.61 1463 CA ASP 214 2742 2095 2993 -117 -898 - 379 MOTA ANISOU 1463 CA ASP 214 16.994 18.030 63.226 1.000 20.58 214 2373 2525 2923 182 -169 -ATOM 1464 C ASP ANISOU 1464 C ASP -169 - 237

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1465 0
                   ASP 214 18.018 18.430 62.678 1.000 23.02
                   ASP 214 2461
ANISOU 1465 O
                                        2883
                                                  3404
                                                          -167 -52 -572
                         214 17.205 18.058 65.637 1.000 23.54
         1466 CB ASP
ANISOU 1466 CB ASP
                          214 3304
                                        2607
                                                  3032
                                                           -92
                                                                  -748 - 668
         1467 CG ASP
ATOM
                          214 16.915 17.506
                                                 67.004 1.000 24.93
ANISOU 1467 CG ASP
                          214 3545
                                        2850
                                                  3079
                                                          450
                                                                  -417 -614
        1468 OD1 ASP
                          214 16.357 16.395
                                                 67.113 1.000 29.17
ANISOU 1468 OD1 ASP
                          214 4134
                                        3070
                                                  3878
                                                          202
                                                                 -705 2 6 2
       1469 OD2 ASP
                          214 17.276 18.191 67.990 1.000 34.38
ANISOU 1469 OD2 ASP
                          214 6917
                                        3040
                                                  3107
                                                        1017 -1413 -736
                          215 15.802 18.452 62.859 1.000 20.74
MOTA
         1470 N
                   LEU
ANISOU 1470 N
                          215 2426
                   LEU
                                        2372
                                                  3081
                                                        86 -60 3 0 6
         1471 CA LEU
MOTA
                          215 15.568 19.401 61.796 1.000 20.55
ANISOU 1471 CA LEU
                         215 2895 2013
                                                  2899
                                                        -202 -178 1 4 1
         1472 C
MOTA
                   LEU
                          215 14.724 20.552 62.332 1.000 19.02
ANISOU 1472 C
                   LEU
                          215 2482 2240
                                                  2504
                                                        -142 -34 321
         1473 0
MOTA
                   LEU
                          215 13.510 20.613 62.142 1.000 22.39
ANISOU 1473 O
                    LEU
                          215 2635
                                        2483
                                                  3389
                                                         -160 -475 5 7 3
         1474 CB LEU
ATOM
                          215 14.826 18.722 60.650 1.000 22.04
                          215 2778 2510 3086 -140 -261 -
215 15.598 17.502 60.128 1.000 25.25
ANISOU 1474 CB LEU
                                                  3086 -140 -261 - 65
         1475 CG LEU
ATOM
ANISOU 1475 CG LEU
                          215 3680
                                        2829
                                                  3085 85 -166 -402
                         215 14.680 16.736 59.174 1.000 27.12
MOTA
         1476 CD1 LEU
ANISOU 1476 CD1 LEU
                         215 4886
                                        2934
                                                  2482
                                                           419
                                                                 -1128 - 65
                         215 16.881 18.046 59.510 1.000 30.76
ATOM
         1477 CD2 LEU
                         215 3434 3089 5165 1003 524 5
216 15.383 21.433 63.078 1.000 19.68
ANISOU 1477 CD2 LEU
                                                          1003 524 561
ATOM
         1478 N
                    PRO
ANISOU 1478 N
                    PRO
                         216 2407
                                        2191
                                                  2879
                                                          -157 148 103
ATOM 1479 CA PRO 216 14.665 22.534 63.708 1.000 22.42
ANISOU 1479 CA PRO 216 2869 2812 2836 272 10 - 22
ATOM 1480 C PRO 216 14.201 23.576 62.698 1.000 25.36
                                                                  10 -228
ANISOU 1480 C PRO 216 4118 2433
ANISOU 1480 C PRO 216 4118 2433 3086 566 -131 -3
ATOM 1481 O PRO 216 14.700 23.759 61.586 1.000 24.67
ANISOU 1481 O PRO 216 3682 2406 3284 187 -176 -2
ATOM 1482 CB PRO 216 15.693 23.092 64.676 1.000 23.88
ANISOU 1482 CB PRO 216 3108 3049 2917 -216 116 -3
ATOM 1483 CG PRO 216 17.033 22.701 64.146 1.000 28.31
ANISOU 1483 CG PRO 216 2994 2996 4766 -88 -117 -1
ATOM 1484 CD PRO 216 2353 1777 5197 -436 -83 -3
ANISOU 1485 N TYR 217 13.154 24.287 63.102 1.000 24.13
ANISOU 1485 N TYR 217 3237 2704 3229 244 -631 -5
                                                  3086
                                                           566 -131 - 315
                                                                -176 - 2 6
                                                          -216 116 -318
                                                                 -117 -1454
                                                          -436 -83 -348
                          217 3237 2704 3229 244 -631 -
217 12.676 25.510 62.462 1.000 26.08
                                                                  -631 - 511
         1486 CA TYR
MOTA
                         217 2514 2899 4498 104 -592 3
217 13.824 26.516 62.369 1.000 25.24
217 3049 2948 3592 -257 -506 -
217 14.570 26.675 63.340 1.000 31.78
ANISOU 1486 CA TYR
                                                                 -592 3 9
MOTA
         1487 C
                    TYR
ANISOU 1487 C
                    TYR
                                                          -257 -506 -538
ATOM
         1488 0
                    TYR
                         217 4114 2863 5096 -332 227
217 11.559 26.103 63.315 1.000 25.97
2773 4346 86 -615 -16
ANISOU 1488 O
                    TYR
                                                          -352 -2151 564
         1489 CB TYR
ANISOU 1489 CB TYR 217 2747
                                                          86 -615 -167
         1490 CG TYR 217 11.189 27.543
                                                 63.125 1.000 31.64
ANISOU 1490 CG TYR
                         217 3080
                                        2803
                                                  6139
                                                           338
                                                                  -1473
ATOM
         1491 CD1 TYR
                         217 10.430 27.928
                                                 62.022 1.000 27.85
ANISOU 1491 CD1 TYR
                         217 2238
                                        3029
                                                                  -175 9
                                                  5314
                                                           511
         1492 CD2 TYR
ATOM
                         217 11.512 28.522
                                                 64.069 1.000 38.49
ANISOU 1492 CD2 TYR
                         217 4721
                                        2813
                                                  7093
                                                          -686 -1682 -749
         1493 CE1 TYR
                          217 10.021 29.219
                                                 61.772 1.000 26.53
ANISOU 1493 CE1 TYR
                          217 1908
                                        2675
                                                  5496 -41
                                                                  107 6 9
         1494 CE2 TYR
                         217 11.113 29.835
                                                 63.827 1.000 42.90
ANISOU 1494 CE2 TYR
                          217 7112
                                        2347
                                                          -1415 -1949 -218
                                                  6842
ATOM
         1495 CZ TYR
                          217 10.373 30.168 62.712 1.000 34.93
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					- 62 -			
ANISOU	1495	CZ	TYR	217 4042	2747	6483	-1462	-545 1 6 6
ATOM	1496		TYR	217 9.996	31.486			36.41
ANISOU			TYR	217 5499	2895	5439	-753	-250 -289
ATOM	1497		ARG	218 14.02		61.218		25.58
ANISOU ATOM	1497		ARG	218 3461	2406	3852	-227	-533 - 476
ANISOU			ARG ARG	218 14.92 218 3630	3 28.243 3270			29.26
ATOM	1499		ARG	218 14.11		4219	-784 1 000	-1349 268 24.81
ANISOU			ARG	218 4063	2949	2415	-382	-228 - 5 6
ATOM	1500		ARG	218 13.74			1.000	29.56
ANISOU			ARG	218 6298	2267	2666	-890	-994 1 6 5
ATOM	1501		ARG	218 16.16			1.000	35.90
ANISOU ATOM	1501		ARG ARG	218 3223 218 17.36	3685	6732	-624	-703 8 9 6
ANISOU			ARG	218 4740	9 28.665 6768	8015	1.000	51.38
ATOM	1503		ARG	218 18.53			1 000	430 - 183 38.84
ANISOU			ARG		6308	3482	-3596	-1165 1647
ATOM	1504		ARG	218 19.34			1.000	45.09
ANISOU			ARG	218 4655	7495	4982	-2325	-962 - 94
ATOM ANISOU	1505 1505		ARG	218 20.27		58.959	1.000	55.53
ATOM	1506		ARG	218 5299 218 20.28	11458 9 28.158		-2701	-1188 -1948
ANISOU	1506	NH1	ARG	218 2399	16648	4071	_19/3	60.85 -1333 548
ATOM	1507	NH2	ARG	218 21.06				60.37
ANISOU	1507	NH2		218 8580	10111	4247		639 - 4241
ATOM	1508	N	PRO	219 13.87			1.000	25.89
ANISOU ATOM	1508		PRO PRO	219 2625	4126	3086	35 29	6 - 1014
ANISOU			PRO	219 13.06 219 2828	31.548 3120			28.10
ATOM	1510		PRO	219 13.63	5 31.959		-410 1 000	379 - 696 28.43
ANISOU			PRO	219 3141	3010	4653	-190	116 - 328
ATOM	1511		PRO	219 12.90				34.17
ANISOU ATOM			PRO	219 4734	3500	4750	302	-798 - 893
ANISOU	1512 1512		PRO PRO	219 13.11 219 5621	32.717 3612	61.316		39.70
ATOM	1513		PRO	219 13.36	3012	5852	-500 1 000	1615 - 1527 42.38
ANISOU			PRO	219 6139	5277	4688	-257	2084 - 2086
ATOM	1514		PRO	219 14.37	30.943			32.77
ANISOU	1514		PRO	219 3901	5719	2831	-602	828 -1603
ATOM ANISOU	1515		ASP	220 14.95				25.65
	1516		ASP	220 3328	1582	4837	-276	801 - 878
ANISOU	1516		ASP	220 15.59 220 3594	2115	4341	-782	248 - 861
ATOM	1517	С	ASP	220 15.78				28.46
ANISOU			ASP	220 3549	1843	5423	-111	1638 - 943
ATOM	1518		ASP	220 16.43				25.80
ANISOU ATOM	1518		ASP	220 3249	2021	4533	-140	
ANISOU	1519	CB	ASP ASP	220 16.91 220 2351	1 32.962 35 3 9	57.998 6938	1.000 - 445	33.76
ATOM	1520		ASP	220 2331	2 31.913			1187 - 1724 42.36
ANISOU	1520	CG	ASP	220 2653	3531	9912	-812	230 - 957
ATOM	1521	OD1	ASP	220 17.48	4 31.170			37.00
ANISOU				220 3154	4148	6757	-104	-410 -2001
ATOM ANISOU	1522	OD2	ASP	220 18.98				37.34
ATOM	1523		ALA	220 2520 221 15.29	4700 2 30.072	6969		24 -1266 24.79
ANISOU			ALA	221 4148	1872	3398		671 - 659
ATOM	1524	CA	ALA	221 15.69	5 29.016			19.17
ANISOU	1524	CA	ALA	221 2165	1868	3251	-52	-92 -610
ATOM	1525		ALA	221 14.55		55.479	1.000	18.60
ANISOU	T272	C	ALA	221 1920	2238	2908	-82	-207 - 362

- 63 -ATOM 1526 0 ALA 221 13.763 27.852 56.415 1.000 26.47 ANISOU 1526 O ALA 221 4127 3289 2641 -1307 894 - 904 1527 CB ALA 221 16.939 28.316 56.104 1.000 19.36 ANISOU 1527 CB ALA 221 2054 2333 2969 -537 -316 6 6 1528 N VAL 222 14.490 27.385 54.313 1.000 17.35 ANISOU 1528 N VAL 222 2089 1841 2661 -101 -323 - 154 1529 CA VAL 222 13.556 26.276 54.083 1.000 17.45 ANISOU 1529 CA VAL 222 1620 2004 3004 -66 -417 1 9 VAL 222 14.333 24.965 54.077 1.000 15.69 MOTA 1530 C ANISOU 1530 C VAL 222 1616 1876 2471 -269 -349 - 324 MOTA 1531 0 VAL 222 15.512 24.934 53.716 1.000 17.84 ANISOU 1531 O VAL 222 1658 1730 3390 -108 -194 4 8 1532 CB VAL 222 12.822 26.433 52.747 1.000 19.60 MOTA ANISOU 1532 CB VAL 222 2267 2202 2979 91 -666 1533 CG1 VAL 222 13.781 26.363 51.563 1.000 21.96 MOTA ANISOU 1533 CG1 VAL 222 2252 3113 2977 250 -645 -182 1534 CG2 VAL 222 11.730 25.411 52.490 1.000 22.44 ATOM ANISOU 1534 CG2 VAL 222 2923 2537 3067 -497 -898 4 4 MOTA 1535 N LEU 223 13.789 23.892 54.621 1.000 16.30 ANISOU 1535 N LEU 223 1792 1694 2706 -239 -93 -532 ATOM 1536 CA LEU ANISOU 1536 CA LEU 223 14.407 22.575 54.579 1.000 15.91 223 1679 1864 2503 -93 -297 -333 ATOM 1537 C 223 14.114 21.908 53.243 1.000 14.86 LEU ANISOU 1537 C 223 1337 1537 2773 -141 -322 -223 12.969 21.888 52.766 1.000 16.23 LEU 1537 2773 -141 -322 - 458 1538 0 ATOM LEU ANISOU 1538 O 223 1317 2132 2719 70 -391 -28 223 13.829 21.779 55.761 1.000 19.97 223 2740 1945 2901 -121 205 -LEU 2132 2719 70 -391 -281 ATOM1539 CB LEU ANISOU 1539 CB LEU 1945 2901 -121 205 -212 223 14.298 20.348 55.882 1.000 23.01 1540 CG LEU ATOM ANISOU 1540 CG LEU 223 2668 1871 4205 -375 -170 9 1 1541 CD1 LEU 223 15.797 20.322 56.143 1.000 23.73 ATOM ANISOU 1541 CD1 LEU 223 2570 3067 3378 69 135 3 1 6 1542 CD2 LEU 223 13.492 19.668 56.979 1.000 35.71 ATOM ANISOU 1542 CD2 LEU 223 2813 3296 7459 525 1116 2333 ATOM 1543 N VAL 224 15.115 21.370 52.570 1.000 14.18 ANISOU 1543 N VAL 224 1383 1446 2560 -28 -320 - 205 1544 CA VAL 224 14.956 20.627 51.330 1.000 14.52 ATOM ANISOU 1544 CA VAL 224 1585 1501 2431 -23 -323 -127 MOTA 1545 C VAL 224 15.320 19.160 51.561 1.000 13.59 ANISOU 1545 C VAL 224 1464 1522 2178 23 -290 -251 1546 0 MOTA VAL 224 16.442 18.861 51.981 1.000 15.38 0 -505 -374 -461 -108 -159 - 408 - 4212863 6 -509 8 7 PHE 1550 N ATOM 225 14.340 18.299 51.299 1.000 13.49 ANISOU 1550 N PHE 225 1494 1526 2106 -66 -353 - 130 1551 CA PHE ATOM 225 14.647 16.882 51.162 1.000 14.67 ANISOU 1551 CA PHE 225 1639 2431 1505 -115 -61 -283 1552 C 225 14.756 16.533 49.675 1.000 14.27 ATOM PHE ANISOU 1552 C 225 1536 PHE 1533 2352 100 -260 -16.876 48.893 1.000 16.25 -260 - 194 ATOM 1553 0 PHE 225 13.858 ANISOU 1553 O PHE 225 1604 2000 2569 296 -311 - 88 ATOM 1554 CB PHE 225 13.537 15.999 51.749 1.000 15.57 ANISOU 1554 CB PHE 225 1613 1563 2740 -46 2 4 -25 ATOM 1555 CG PHE 225 13.387 15.996 53.257 1.000 17.95 ANISOU 1555 CG PHE 225 1888 2267 2666 -650 -302 2 0 3 ATOM 1556 CD1 PHE 225 14.409 15.809 54.157 1.000 27.39

ANISOU ATOM ANISOU	1155555566666666666666666666667777777777	CCCCCCCCNNCCCCOOCCSSNNCCCCOONNCCCCCOOCCNNCCCCOOCCOO	PPPPPPPPCCCCCCCCCCCCCGGGGGGGGAAAAAAAAAIIIIIIIIII	222222222222222222222222222222222222	12.125 2333 14.211 3108 11.910 2994 12.958 3705 15.795 1428 15.810 13.60 14.903 15.33 14.961 18.224 14.150 13.88 13.352 1279 13.903 15.81 14.917 1630 13.663 14.917 1630 13.663 14.98 15.666 14.482 17.714 1808 12.909 1340	2765 15.673 3657 10 2414 15.787 3716 15.817 129.180 1440 13.956 1212 13.217 165.85 16.367 1740 13.722 14.855 16.367 1740 13.722 15.313 11.541	5291.52486.31.668.524.3.1.653.	1.000 21.09 -166 399 -527 1.000 26.82 -1044 -1241 1128 1.000 21.65 623 239 - 39 1.000 28.82 -832 -663 3 4 0 1.000 12.77 -60 -370 - 239 1.000 12.99 12 -355 - 207 1.000 12.37 8 -283 - 311 1.000 15.68 -140 -611 158 1.000 13.77 19 -203 - 75 1.000 16.37 -222 -236 - 12 1.000 13.20 -28 -293 - 290 1.000 12.58 -83 -438 - 255 1.000 12.54 15 -288 - 79 1.000 13.58 51 -155 8 2 1.000 13.58 51 -155 8 2 1.000 13.02 59 -204 - 161 1.000 12.41 -68 -119 - 63 1.000 12.82 97 -223 - 5 1.000 13.64 26 -6 - 131 1.000 14.56 -219 358 - 243 1.000 13.61

	- 65 -	
ATOM 1587 O AL.		41 146 1 000 12 65
ANISOU 1587 O AL		41.146 1.000 13.65 2418 108 4 4 6
ATOM 1588 CB AL.		43.345 1.000 13.66
ANISOU 1588 CB AL		2215 -186 -21 -229
ATOM 1589 N TH		42.805 1.000 13.31
ANISOU 1589 N TH	R 231 1526 1318	2214 58 -261 - 1
ATOM 1590 CA TH		42.659 1.000 13.32
ANISOU 1590 CA TH		2093 78 -302 3 2
ATOM 1591 C THE ANISOU 1591 C THE		41.251 1.000 13.27
ANISOU 1591 C THE ATOM 1592 O THE		2111 205 -211 3
ANISOU 1592 O TH		40.620 1.000 15.51
ATOM 1593 CB TH		2667 245 58 - 170
ANISOU 1593 CB TH		43.688 1.000 13.03 2151 46 -166 1 2
ATOM 1594 OG1 TH	R 231 17.530 9.313	44.995 1.000 14.70
ANISOU 1594 OG1 TH	R 231 1742 1614	2230 -99 32 -14
ATOM 1595 CG2 TH		43.697 1.000 13.69
ANISOU 1595 CG2 TH	R 231 1449 1419	2335 113 -211 1 9 7
ATOM 1596 N LET ANISOU 1596 N LET		40.796 1.000 13.43
ANISOU 1596 N LEG ATOM 1597 CA LEG		2271 75 -404 - 27
ANISOU 1597 CA LET		39.527 1.000 14.11
ATOM 1598 C LET		2326 80 -468 4 9 38.381 1.000 15.53
ANISOU 1598 C LEG		2376 209 -3 9 0
ATOM 1599 O LET	U 232 17.749 8.808	37.504 1.000 17.16
ANISOU 1599 O LET	U 232 2024 1949	2546 107 -116 - 519
ATOM 1600 CB LET		39.368 1.000 14.47
ANISOU 1600 CB LET ATOM 1601 CG LET		2175 72 -396 -161
ATOM 1601 CG LET ANISOU 1601 CG LET		38.155 1.000 15.89
ATOM 1602 CD1 LET	U 232 1941 1768 U 232 15.118 5.920	2329 120 -470 -303
ANISOU 1602 CD1 LEG	U 232 3565 2020	38.202 1.000 23.19 3228 743 -1110 -851
ATOM 1603 CD2 LET	U 232 13.003 7.190	38.126 1.000 19.46
ANISOU 1603 CD2 LET	U 232 2006 2262	3126 -470 -523 - 66
ATOM 1604 N VAI		38.299 1.000 13.73
ANISOU 1604 N VAI		2025 -7 -263 193
ATOM 1605 CA VAI ANISOU 1605 CA VAI		37.117 1.000 13.84
ANISOU 1605 CA VAI ATOM 1606 C VAI		1926 141 -73 1 0 7
ANISOU 1606 C VA	T 000 4046	37.025 1.000 14.08 1958 72 -46 1 1 3
ATOM 1607 O VAI		1958 72 -46 1 1 3 35.910 1.000 16.65
ANISOU 1607 O VAI		2079 38 109 4 0 1
ATOM 1608 CB VA	L 233 16.098 12.626	37.062 1.000 14.69
ANISOU 1608 CB VAI		2206 141 -165 3 3 3
ATOM 1609 CG1 VAI		38.113 1.000 15.70
ANISOU 1609 CG1 VAI ATOM 1610 CG2 VAI		2698 34 156 - 28
ANISOU 1610 CG2 VAI	20.200	35.647 1.000 16.43
ATOM 1611 N TH		2459 251 117 5 9 6 38.175 1.000 14.23
ANISOU 1611 N THI		2083 146 -110 2 3 5
ATOM 1612 CA THI	R 234 20.524 11.908	38.148 1.000 16.14
ANISOU 1612 CA THI	R 234 1664 1868	2602 63 -171 - 4 9
ATOM 1613 C THI		38.006 1.000 17.09
ANISOU 1613 C THI ATOM 1614 O THI		2912 146 211 - 51
ATOM 1614 0 THI ANISOU 1614 0 THI		38.139 1.000 17.25
ATOM 1615 CB THI		2828
ANISOU 1615 CB TH	R 234 1667 1502	2642 -46 -149 1 6 3
ATOM 1616 OG1 TH	R 234 20.849 11 819	40.522 1.000 15.45
ANISOU 1616 OG1 TH	R 234 1659 1708	2502 -80 59 4 4
ATOM 1617 CG2 TH	R 234 20.291 13.978	39.597 1.000 16.61

W O 33155774	00	
1618 888	- 66 -	
ANISOU 1617 CG2 THR	234 1564 1672	3077 3 -34 - 42
ATOM 1618 N GLY	235 20.712 9.441	37.833 1.000 15.80
ANISOU 1618 N GLY	235 1905 1914	2564 193 29 - 219 37.792 1.000 17.10
ATOM 1619 CA GLY ANISOU 1619 CA GLY	235 21.484 8.209 235 2049 1861	
ANISOU 1619 CA GLY ATOM 1620 C GLY	235 2049 1861 235 22.225 7.931	2586 133 223 -488 39.083 1.000 18.06
ANISOU 1620 C GLY	235 22.225 7.931	2768 419 499 3 0 3
ATOM 1621 0 GLY	235 23.285 7.289	39.010 1.000 21.26
ANISOU 1621 O GLY	235 2167 2606	3303 679 343 - 74
ATOM 1622 N GLY		40.237 1.000 16.17
ANISOU 1622 N GLY	236 1663 1901	2582 36 291 3 0 5
ATOM 1623 CA GLY	236 22.080 7.673	41.520 1.000 17.27
ANISOU 1623 CA GLY	236 2135 1671	2754 225 28 2 2 9
ATOM 1624 C GLY		42.194 1.000 16.88
ANISOU 1624 C GLY	236 1880 1890	2644 204 100 222
ATOM 1625 O GLY	236 23.692 8.272	43.193 1.000 19.42
ANISOU 1625 O GLY	236 2165 2399	2814 314 -90 419
ATOM 1626 N GLN	237 23.134 9.890	41.746 1.000 16.99
ANISOU 1626 N GLN	237 1647 1851	2957 213 -213 1 6 7
ATOM 1627 CA GLN ANISOU 1627 CA GLN		42.298 1.000 16.75 2752 72 177 9 8
ATOM 1628 C GLN	237 1608 2004 237 23.481 11.604	
ANISOU 1628 C GLN	237 1404 2136	
ATOM 1629 0 GLN	237 24.183 12.382	
ANISOU 1629 O GLN	237 1581 2508	
ATOM 1630 CB GLN	237 24.456 11.855	41.217 1.000 17.17
ANISOU 1630 CB GLN	237 1912 2080	
ATOM 1631 CG GLN	237 25.304 11.221	
ANISOU 1631 CG GLN	237 1850 2410	
ATOM 1632 CD GLN	237 25.721 12.302	39.137 1.000 19.72
ANISOU 1632 CD GLN ATOM 1633 OE1 GLN	237 1680 2833 237 26.602 13.110	2979 104 317 3 0 7 39.436 1.000 24.27
ATOM 1633 OE1 GLN ANISOU 1633 OE1 GLN	237 26.602 13.110 237 1841 3145	
ATOM 1634 NE2 GLN	237 24.986 12.399	
ANISOU 1634 NE2 GLN	237 2007 2298	
ATOM 1635 N VAL	238 22.221 11.359	
ANISOU 1635 N VAL	238 1563 1804	
ATOM 1636 CA VAL	238 21.533 12.075	44.862 1.000 14.41
ANISOU 1636 CA VAL	238 1535 1553	
ATOM 1637 C VAL	238 20.861 11.060	
ANISOU 1637 C VAL	238 1414 1392	
ATOM 1638 O VAL	238 20.136 10.174	
ANISOU 1638 O VAL ATOM 1639 CB VAL	238 1655 1639 238 20.467 13.061	
ANISOU 1639 CB VAL	238 1817 1626	2152 35 -437 - 95
ATOM 1640 CG1 VAL	238 19.805 13.764	
ANISOU 1640 CG1 VAL	238 1965 1490	2510 174 -524 - 423
ATOM 1641 CG2 VAL	238 21.064 13.994	
ANISOU 1641 CG2 VAL		2812 -60 -378 2 2 2
ATOM 1642 N LYS	239 21.119 11.153	
ANISOU 1642 N LYS	239 1704 1474	2318 14 -40 1 2
ATOM 1643 CA LYS	239 20.470 10.360	
ANISOU 1643 CA LYS		2406 106 -168 1 7 9
ATOM 1644 C LYS ANISOU 1644 C LYS		48.409 1.000 14.82 2642 102 -53 232
ATOM 1645 0 LYS		
ANISOU 1645 O LYS		2318 158 -275 1 9 0
ATOM 1646 CB LYS		
ANISOU 1646 CB LYS	239 1995 1712	2527 243 -543 2 5 2
ATOM 1647 CG LYS	239 20.767 9.549	50.498 1.000 16.65
ANISOU 1647 CG LYS	239 1954 1759	2614 -58 -781 2 4 4

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ATOM	1648	CD	LYS	230	21.738	9.511	E1 (0)	1 000	10 56
ANISOU			LYS		2954	1820	2732	-123	19.76 -1234 363
ATOM	1649	CE	LYS		21.107	8.835	52.896		
ANISOU			LYS	239	3331	2164	3086	-652	-1502 8 6 3
ATOM	1650	NΖ	LYS	239	21.904	8.883	54.145		23.13
ANISOU			LYS		2817	3360	2612	-471	-943 2 8 7
ATOM ANISOU	1651		ALA	240		9.892	48.659		
ATOM	1652		ALA ALA		1429 16.791	1607	2418	-156	-334 - 61
ANISOU			ALA	240	1468	10.192 1635	49.145 2210	1.000	13.98
ATOM	1653		ALA		16.728	9.776	50.605	-151	
ANISOU			ALA		1439	1388	2279	77 -45	13.44
ATOM	1654		ALA	240	16.514	8.592			16.32
ANISOU			ALA		1932	1567	2699	-215	-673 3 1 4
ATOM ANISOU	1655		ALA		15.712	9.565	48.268	1.000	15.21
ANISOU	1656		ALA PRO		1510	1962	2306	-104	-387 - 307
ANISOU			PRO		16.907 1634	10.701 1551	51.546	1.000	
ATOM	1657		PRO		17.035	10.251	2221 52.940	-87	-292 7 1
ANISOU	1657	CA	PRO		1718	1681	2180	-350	-174 - 30
ATOM	1658		PRO	241	15.693	9.961	53.579		
ANISOU			PRO		1659	1581	2039	-107	-207 - 74
ATOM	1659		PRO		14.629	10.527	53.261		
ANISOU ATOM	1660		PRO PRO		1698 17.689	1946	2838	17 -25	
ANISOU			PRO		2162	11.462 1657	53.619		
ATOM	1661	_	PRO		17.138	12.651	2501 52.826	-460 1 000	-487 5 5
ANISOU	1661	CG	PRO		2433	1601	2258	-367	-274 3 1
MOTA	1662		PRO		17.164	12.140	51.409		
	1662		PRO		1841	1490	2339	-215	-186 - 66
ATOM	1663 1663		ARG		15.740	9.049	54.544		
ANISOU ATOM	1664		ARG ARG		1914	1853	2212		-308 2 0 4
	1664		ARG		14.574 1955	8.772 1863	55.376		
ATOM	1665		ARG		14.406	9.841	2073 56.437	-236 1 000	-291 1 8 0
ANISOU			ARG		1889	2011	2407		-411 - 51
ATOM	1666		ARG		15.372	10.416	56.994	1.000	18.31
ANISOU			ARG		2041	2186	2732	-216	-559 - 180
ATOM ANISOU	1667		ARG		14.728	7.419	56.085		
ATOM	1668		ARG ARG		2920 14.564	1810	2253	-486	-391 2 6 9
ANISOU	1668	CG	ARG		2372	6.273 1873	55.094 2755	1.000	18.42
ATOM	1669	CD	ARG		14.854	4.935	55.796		162 - 155
ANISOU			ARG		3380	2022	3366	470	-483 - 217
ATOM	1670	ΝE	ARG	242	16.334	4.954	55.991		
ANISOU			ARG		3498	2727	3916	444	-829 4 7
ATOM ANISOU	1671	CZ	ARG	242	16.941	3.921	56.584		
ATOM	1672		ARG		3166 16.157	2879	4284	-297	-1143 8 0 2
ANISOU	1672	NHI	ARG	242	3810	2.913 3235	56.989 5546		
ATOM	1673	NH2	ARG		18.241	3.889	56.779		
ANISOU	1673	NH2	ARG	242	3043	2925	5859	227	-769 4 8 4
ATOM	1674	N	HIS	243	13.188	10.057	56.872		17.55
ANISOU			HIS		1979	2233	2457	-165	-173 - 74
ATOM ANISOU	1675 1675		HIS HIS		12.913	11.050	57.914		
ATOM	1676		HIS		2186 11.644	2139 10.627	2452	-260	-123 - 75
ANISOU			HIS		2102	2084	58.643 2470		17.52 -164 - 325
ATOM	1677	0	HIS		10.870	9.803	58.132	1.000	204 - 3 4 5
ANISOU	1677	0	HIS	243	2226	2593	2868		-323 - 392
ATOM	1678	CB	HIS	243	12.865	12.456	57.324	1.000	19.74

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ANISOU 1678 CB HIS 243 2770 2248 2482 -188 -106 8 ATOM 1679 CG HIS 243 11.922 12.630 56.187 1.000 22.60 ANISOU 1679 CG HIS 243 3449 2513 2624 164 -382 0 ATOM 1680 ND1 HIS 243 12.209 12.299 54.879 1.000 25.87 ANISOU 1680 ND1 HIS 243 4780 2575 2473 -609 -403 5 -188 -106 8 3 243 4780 2575 2473 -609 -403 5 243 10.633 13.034 56.172 1.000 29.11 243 3220 4490 3348 121 -421 1 -609 -403 5 3 ATOM 1681 CD2 HIS ANISOU 1681 CD2 HIS 243 3220 4490 3348 121 -421 1 243 11.182 12.573 54.109 1.000 32.92 -421 1630 1682 CE1 HIS ANISOU 1682 CE1 HIS 243 5835 3672 3001 -1102 -1367 689 243 10.214 13.012 54.875 1.000 36.95 1683 NE2 HIS ANISOU 1683 NE2 HIS 243 5719 4201 4119 1019 -2016 987 244 11.437 11.194 59.831 1.000 18.87 ATOM 1684 N HIS ANISOU 1684 N HIS 244 2523 2477 2171 -88 -141 - 117244 10.302 10.801 60.649 1.000 20.83 1685 CA HIS MOTA 244 2802 244 9.927 ANISOU 1685 CA HIS 2485 2628 171 251 272 1686 C HIS 11.968 61.551 1.000 20.33 ATOM ANISOU 1686 C HIS 244 1803 2969 2953 -31 ATOM 1687 O HIS 244 10.482 13.073 61.510 1.000 21.71 ANISOU 1687 O HIS 244 2057 3418 2774 -535 145 -1 ATOM 1688 CB HIS 244 10.714 9.557 61.468 1.000 24.38 ANISOU 1688 CB HIS 244 4066 2644 2553 -76 -390 4 -78 145 - 853 ANISOU 1688 CB HIS ATOM 1689 CG HIS ANISOU 1689 CG HIS 1688 CB HIS 244 4066 2644 2553 -76 -390 4 4 1 1689 CG HIS 244 11.859 9.725 62.423 1.000 28.34 1689 CG HIS 244 4158 3498 3113 696 -727 - 8 9 1690 ND1 HIS 244 13.132 9.205 62.268 1.000 32.35 1690 ND1 HIS 244 4012 4471 3808 548 -485 - 8 5 0 1691 CD2 HIS 244 11.928 10.391 63.609 1.000 25.21 1691 CD2 HIS 244 2937 4137 2505 -373 45 2 1 9 1692 CE1 HIS 244 13.887 9.531 63.312 1.000 31.71 1692 CE1 HIS 244 4157 4277 3613 1224 -749 -5 1 8 1693 NE2 HIS 244 13.146 10.263 64.150 1.000 24.52 1693 NE2 HIS 244 3165 3517 2633 94 -82 4 9 2 1694 N VAL 245 8.890 11.687 62.349 1.000 23.87 1694 N VAL 245 8.890 11.687 62.349 1.000 23.87 1695 CA VAL 245 8.473 12.691 63.349 1.000 24.85 1695 CA VAL 245 2785 3770 2888 481 149 -293 ATOM ANISOU 1690 ND1 HIS ATOM ANISOU 1691 CD2 HIS ATOM ANISOU 1692 CE1 HIS ATOM ANISOU 1693 NE2 HIS ATOM ANISOU 1694 N ATOM ANISOU 1695 CA VAL 245 2785 3770 2888 481 149 - 293 VAL 245 2785 3770 2888 481 149 - VAL 245 8.624 12.079 64.735 1.000 26.03 ATOM 1696 C ANISOU 1696 C VAL 245 3220 3558 3112 -289 179 8 9 3558 3112 -289 1/9 8 11.025 64.969 1.000 27.98 ATOM 1697 0 VAL 245 8.023 ANISOU 1697 O VAL 245 3120 3085 4428 42 295 - 59 ATOM 1698 CB VAL 245 7.020 13.114 63.099 1.000 26.02 ANISOU 1698 CB VAL 245 2621 3489 3777 94 -103 -56
ATOM 1699 CG1 VAL 245 6.586 14.114 64.161 1.000 28.06
ANISOU 1699 CG1 VAL 245 2717 3330 4614 159 746 -2
ATOM 1700 CG2 VAL 245 6.927 13.705 61.680 1.000 30.51
ANISOU 1700 CG2 VAL 245 3564 3809 4220 1264 -305 -1
ATOM 1701 N ALA 246 9.399 12.696 65.603 1.000 28.08
ANISOU 1701 N ALA 246 4338 3787 2543 -850 250 23
ATOM 1702 CA ALA 246 4363 3787 2543 -850 250 23
ATOM 1702 CA ALA 246 4363 3360 2707 292 275 3
ATOM 1703 C ALA 246 4363 3360 2707 292 275 3
ATOM 1703 C ALA 246 8.356 12.740 67.833 1.000 32.68
ANISOU 1703 C ALA 246 4915 4473 3031 98 880 197
ATOM 1704 O ALA 246 7.774 13.791 67.563 1.000 29.54
ANISOU 1704 O ALA 246 3522 4283 3417 -224 875 -1
ATOM 1705 CB ALA 246 10.819 13.010 67.542 1.000 30.33
ANISOU 1705 CB ALA 246 4564 3949 3011 615 -221 -4 ANISOU 1698 CB VAL 245 2621 3489 3777 94 -103 -569 4614 159 746 -485 4220 1264 -305 - 33 -850 250 254 275 373 **-224** 875 **-329** ANISOU 1705 CB ALA 246 4564 3949 3011 615 -221 -11.958 68.849 1.000 34.09 -221 - 422 ALA 247 8.048 1706 N ANISOU 1706 N ALA 247 4483 5156 3311 -1190 466 3 12.190 69.859 1.000 34.23 5156 -1190 466 3 9 3 1707 CA ALA 247 7.036 ANISOU 1707 CA ALA 247 4188 5627 3189 -1215 315 515 MOTA 12.910 71.081 1.000 33.31 1708 C ALA 247 7.609 ANISOU 1708 C 4684 ALA 247 5419 2555 249 -506 1147

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ANISOU 1709 O ATOM 1710 CB ANISOU 1710 CB ANISOU 1711 N ANISOU 1711 N ATOM 1712 CA ANISOU 1713 C ANISOU 1713 C ANISOU 1714 O ANISOU 1715 CB ANISOU 1715 CB ANISOU 1716 CG ANISOU 1716 CG ANISOU 1717 CD ANISOU 1717 CD ANISOU 1718 N ATOM 1718 N ATOM 1719 CA ANISOU 1719 CA ANISOU 1720 C ANISOU 1721 O ATOM 1721 CD ATOM 1721 CD ANISOU 1722 CB ANISOU 1722 CB ANISOU 1723 CG ANISOU 1724 CD ANISOU 1724 CD ANISOU 1725 NE ATOM 1725 NE ANISOU 1726 CZ ANISOU 1727 NH1 ANISOU 1728 NH2 ANISOU 1728 NH2 ANISOU 1729 N ANISOU 1731 C ANISOU 1732 CA ANISOU 1733 CB ANISOU 1733 CB ANISOU 1733 CB ANISOU 1734 N ANISOU 1735 CA	ARG 249 22286 ARG 249 12.682 ARG 249 5358 ALA 254 1.981 ALA 254 15501 ALA 254 2.287 ALA 254 12510 ALA 254 2.943 ALA 254 8383 ALA 254 8.174 ALA 254 8056 ALA 254 3.264 ALA 254 12589 GLY 255 8029 GLY 255 2.880	4478 10.881 6726 13.851 5458 15458 14.581 5478 13.61 5478 13.62 71 53.66 12.79 13.66 15.64 15.64 15.64 15.64 15.64 15.64 15.64 15.64 17.16 18.38 12.16 13.82 13.82 13.83 12.16 13.82 13.83 12.16 13.82 13.83 12.71 13.33 12.71 13.33 13.99 16.2 17.10 19.97 17.30 19.97 17.30 19.97 17.30 19.97 18.10 19.97 19.30 19.62 18.10 19.62 19.62 19.62 19.62 19.62 19.62 19.62 19.63 17.63	71.523 1.000 38.23 4259 -378 -1519 1230 70.314 1.000 47.11 2801 -2800 1464 68 6 71.577 1.000 42.28 4836 -300 933 -97 72.773 1.000 44.85 3996 -645 1413 21 4 73.948 1.000 49.25 5075 -1446 552 98 5 74.014 1.000 45.48 4237 -1127 2573 -79 6 72.897 1.000 49.75 5523 -513 1238 -138 72.299 1.000 50.89 6545 -108 2210 -10 64 71.114 1.000 44.69 6006 937 953 -577 74.883 1.000 48.76 3045 -1317 1069 - 477 76.024 1.000 55.51 4156 -1098 895 56 6 76.916 1.000 46.09 3568 -2484 -7 1237 77.831 1.000 55.24 4326 705 2864 1270 76.110 1.000 71.04 6779 1135 3707 622 77.165 1.000 72.89 7984 2171 2723 40 9 76.580 1.000 72.71 7942 2304 2153 133 78.521 1.000 89.50 5559 2015 1622 38 74 76.761 1.000 67.68 10295 1004 3886 22 1 75.430 1.000 85.24 8964 -4581 -1437 23 47 76.257 1.000 72.71 7942 2304 2153 133 78.521 1.000 89.50 5559 2015 1622 38 74 76.761 1.000 67.68 10295 1004 3886 22 1 75.430 1.000 72.71 7942 2304 2153 133 78.521 1.000 89.50 5559 2015 1622 38 74 76.761 1.000 67.68 10295 1004 3886 22 1 75.430 1.000 60.91 9040 -506 2886 13 12 75.487 1.000 72.37 11332 1602 4553 33 81 77.351 1.000 60.48 8286 -3993 1617 15 92 75.489 1.000 72.37 11332 1602 4553 33 81 77.351 1.000 60.48 83131 -866 4570 -1112 74.846 1.000 54.40 7190 594 2922 -940 74.098 1.000 40.05
ANISOU 1733 CB ATOM 1734 N ANISOU 1734 N	ALA 254 12589 GLY 255 2.200 GLY 255 8029	7262 22.108 5451	3131 -866 4570 -1112 74.846 1.000 54.40 7190 594 2922 -940
ATOM 1737 O ANISOU 1737 O ATOM 1738 N ANISOU 1738 N ATOM 1739 CA	GLY 255 4.580 GLY 255 2978 SER 256 3.164 SER 256 5047	23.163 6491 21.387 4594 20.606	72.398 1.000 39.96 5715 -128 -136 -2226 72.509 1.000 37.29 4527 389 11 -853 71.429 1.000 35.71

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ANISOU 1739 CA SER 256 4737 4533 4299 560 -5C1 - 919 256 2.983 20.742 1740 C 70.118 1.000 34.93 ATOM SER ANISOU 1740 C -85 9 1 SER 256 4584 4669 4019 -98 1741 0 256 3.251 69.162 1.000 33.92 ATOM SER 20.000 ANISOU 1741 O SER 256 3575 6107 3207 503 304 377 256 3.845 1742 CB ATOM SER 19.136 71.853 1.000 30.17 ANISOU 1742 CB SER 256 3125 4830 3509 624 212 - 4921743 OG SER 256 2.688 18.752 72.601 1.000 61.15 ANISOU 1743 OG SER 256 2987 8497 11750 451 1943 2630 1744 N 257 2.065 SER 21.700 70.030 1.000 35.54 ATOM ANISOU 1744 N 257 4037 5989 SER 3479 347 242 - 86257 1.379 ATOM 1745 CA SER 257 2824 257 2.378 257 2.1 21.993 68.767 1.000 30.95 ANISOU 1745 CA 5827 170 SER 3109 672 - 509 1746 C SER 22.538 67.760 1.000 30.63 ATOM 257 3181 257 3.359 ANISOU 1746 C SER 5524 2934 -476 765 -1297 1747 0 SER 23.159 68.199 1.000 34.70 257 3500 ANISOU 1747 O SER 6070 3616 -829 603 -1516 257 0.331 1748 CB SER 69.036 1.000 38.70 23.088 MOTA ANISOU 1748 CB SER 257 3085 6518 796 1381 4 3 5 5103 257 0.801 24.361 MOTA 1749 OG SER 68,601 1.000 65.12 11565 -999 -3375 383 ANISOU 1749 OG SER 257 8002 5175 1750 N 258 2.119 22.384 66.471 1.000 30.51 ATOM ARG -332 677 -995 ANISOU 1750 N ARG 258 3668 5068 2855 258 2.997 22.819 65.396 1.000 28.15 ATOM 1751 CA ARG 258 3100 ANISOU 1751 CA ARG 4620 2976 -106 358 -544 258 2.198 22.913 64.096 1.000 25.64 ATOM 1752 C ARG ANISOU 1752 C ARG 258 3488 3381 2872 -676 273 -904 258 1.132 258 3162 258 4 22.294 63.981 1.000 24.93 ATOM 1753 0 ARG 258 1.132 ANISOU 1753 O ARG 3240 3070 -441 478 -560 MOTA 1754 CB ARG 258 4.175 21.873 65.154 1.000 27.21 ANISOU 1754 CB 4041 3141 -446 313 -1352 20.508 64.570 1.000 30.90 258 3158 ARG 1755 CG 258 3.861 ARG ATOM ANISOU 1755 CG ARG 258 4782 3429 3531 -737 -738 - 389 19.537 64.769 1.000 36.65 258 5.039 ATOM 1756 CD ARG ANISOU 1756 CD ARG 258 5937 106 477 306 3466 4523 1757 NE ATOM 258 4.597 18.176 64.411 1.000 32.42 ARG ANISOU 1757 NE ARG 258 3372 3858 5089 -85 -274 5 2 8 MOTA 1758 CZ ARG 258 4.633 17.777 63.143 1.000 37.32 ANISOU 1758 CZ ARG 258 5670 2958 5553 155 680 4 3 1759 NH1 ARG 258 5.075 18.622 62.217 1.000 29.98 ATOM ANISOU 1759 NH1 ARG 258 3077 3435 4881 -150 -211 -103 ATOM 1760 NH2 ARG 258 4.210 ANISOU 1760 NH2 ARG 258 5812 ATOM 1761 N THR 259 2.806 ANISOU 1761 N THR 259 2625 ATOM 1762 CA THR 259 2.337 ANISOU 1762 CA THR 259 2614 ATOM 1763 C THR 259 3.528 16.566 62.824 1.000 38.66 5724 -190 -1632 865 3151 23.572 63.120 1.000 23.62 3578 2771 -519 315 -1037 23.482 61.730 1.000 21.97 2800 2934 -36 247 -1041 23.197 60.808 1.000 19.76 MOTA 1763 C THR 259 3.528 ANISOU 1763 C THR 259 2257 21 - 699 2663 2587 -38 1764 0 MOTA 259 4.698 23.411 61.159 1.000 21.13 THR ANISOU 1764 O 259 2464 THR 3096 2468 -495 -10 -286 MOTA 1765 CB THR 259 1.682 24.793 61.278 1.000 24.04 ANISOU 1765 CB THR 259 2125 3084 3927 70 -157 -1229 1766 OG1 THR 259 2.697 25.790 61.041 1.000 23.14 ANISOU 1766 OG1 THR 259 2297 2848 3648 196 -142 - 8291767 CG2 THR 259 0.760 25.408 62.331 1.000 25.17 264 - 136 ANISOU 1767 CG2 THR 259 2941 3229 3393 726 1768 N MOTA SER 260 3.234 22.706 59.600 1.000 20.41 ANISOU 1768 N SER 260 2386 74 - 806 2762 2609 -61 MOTA 1769 CA SER 260 4.225 22.515 58.551 1.000 19.33 ANISOU 1769 CA 260 2488 2459 SER 2399 192

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					- 71 -		
ATOM	1770	С	SER	260 3.587	22.871	57 210	1.000 18.78
ANISOU	1770	С	SER	260 1996	2544	2595	-379 -264 - 311
ATOM	1771	0	SER	260 2.375	22.758		1.000 21.20
ANISOU	1771	0	SER	260 1917	2448	3689	-75 -269 - 5 7 3
ATOM	1772	СВ	SER	260 4.738	21.076		1.000 20.28
ANISOU	1772	CB	SER	260 2491	2458	2755	160 -101 - 495
ATOM	1773	OG	SER	260 3.656	20.197		1.000 22.70
	1773		SER	260 2758	2574	3294	-113 -284 -169
ATOM	1774		SER	261 4.474	23.329		1.000 18.79
ANISOU			SER	261 2189	2215	2737	-55 - 92 3 5
ATOM	1775	CA	SER	261 4.148	23.585	54.929	-55 -92 3 5 1.000 16.88
ANISOU			SER	261 2074	1718	2622	22 -117 -404
ATOM	1776		SER	261 5.066	22.672		1.000 17.25
ANISOU	1776	С	SER	261 1720	1833	3000	101 -350 - 491
ATOM	1777		SER	261 6.272	22.876	54.173	1.000 19.96
ANISOU	1777	0	SER	261 1712	2417	3456	50 -483 -781
ATOM	1778	CB	SER	261 4.471	25.028		1.000 19.95
ANISOU	1778	CB	SER	261 2903	1675	3002	164 -113 -135
ATOM	1779	OG	SER	261 4.404	25.127	53.107	1.000 35.64
ANISOU	1779	OG	SER	261 5435	4814	3293	-1089 -766 1263
ATOM	1780	N	VAL	262 4.467	21.722		1.000 15.56
ANISOU	1780		VAL	262 1751	2021	2140	-75 -40 -436
MOTA	1781	CA	VAL	262 5.247	20.713		1.000 15.41
ANISOU	1781	CA	VAL	262 1871	1938	2048	43 21 - 196
ATOM	1782	С	VAL	262 4.914	20.874		1.000 14.05
ANISOU			VAL	262 1460	1784	2095	-13 29 - 144
MOTA	1783	0	VAL	262 3.759	20.712		1.000 15.45
ANISOU	1783		VAL	262 1488	1900	2481	-175 -94 -191
ATOM	1784		VAL	262 4.902	19.307	53.253	1.000 16.87
ANISOU	1784		VAL	262 2144	2005	2260	165 -164 2 3
MOTA	1785	CG1	VAL	262 5.567	18.275		1.000 20.01
ANISOU				262 2433	2006	3165	4 -191 -637
ATOM	1786	CG2	VAL	262 5.335	19.200	54.715	1.000 18.63
	1786	CG2		262 2390	2242	2446	147 ~397 1 7 5
ATOM	1787	И	PHE	263 5.894	21.163	50.412	1.000 13.73
	1787		PHE	263 1497	1573	2148	5 -64 1 8 6
MOTA	1788		PHE	263 5.762	21.411	48.994	1.000 13.04
	1788		PHE	263 1654	1196	2105	-12 -193 1 1 3
ATOM	1789		PHE	263 6.479	20.253	48.284	1.000 13.56
	1789		PHE	263 1432	1351	2370	-175 -98 -87
ATOM	1790		PHE	263 7.732	20.177	48.281	1.000 13.83
	1790		PHE	263 1415	1437	2403	-82 -299 -104
ATOM	1791	CB	PHE	263 6.364	22.770	48.594	1.000 13.50
ANISOU			PHE	263 1658	1374	2098	-295 -97 3 4
ATOM	1792		PHE	263 6.062	23.148		1.000 13.34
ANISOU			PHE	263 1616	1358	2096	-159 -111 8 2
ATOM	1793	CD1	PHE	263 6.750	22.635	46.051	1.000 14.95
ANISOU				263 1977	1547	2156	-354 -131 - 384
ATOM	1794	CD2	PHE	263 5.005	24.048		1.000 15.37
ANISOU	1794	CD2	PHE	263 1549	1557	2735	-139 -264 3 0 3
ATOM	1795	CEI	PHE	263 6.468	22.945		1.000 14.58
ANISOU				263 1721	1621	2196	-242 71 -144
ATOM	1796	CE2	PHE	263 4.703	24.366		1.000 14.71
ANISOU ATOM	1707	CE2		263 1482	1428	2680	-20 -261 1 3 7
	1797		PHE	263 5.383	23.809		1.000 16.55
ANISOU ATOM	1798		PHE	263 1935	1492	2862	-152 29 1 4
ANISOU			PHE	264 5.721	19.405		1.000 12.07
ANISOU	1798		PHE	264 1277	1343	1967	-66 -49 1 9
ANISOU			PHE	264 6.267	18.328		1.000 11.90
ATOM	1800		PHE	264 1177	1289	2058	-129 34 - 21
AIOH	7000		PHE	264 6.440	18.775	45.314	1.000 11.76

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1258
ANISOU 1800 C
               PHE 264 1206
                                        2004
                                               -121
                                                     -42 8
                                19.097 44.683 1.000 12.55
               PHE
                    264 5.418
       1801 0
                     264 1165
                                                    -120 4 6
ANISOU 1801 O
                PHE
                                1473
                                               -77
                                        2133
                     264 5.346
                                17.099
                                       46.773 1.000 12.39
       1802 CB PHE
MOTA
ANISOU 1802 CB PHE
                    264 1101
                                1498
                                             -304 -42 6 3
                                        2110
ATOM
       1803 CG
               PHE
                    264 5.022
                                16.558
                                       48.150 1.000 13.97
                                              -290 13 121
ANISOU 1803 CG PHE
                    264 1647
                                1465
                                        2197
ATOM
       1804 CD1 PHE
                     264 5.960
                                15.848 48.852 1.000 17.07
ANISOU 1804 CD1 PHE
                     264 2039
                                1976
                                        2471
                                               -422 -410497
                     264 3.747
                                16.679
       1805 CD2 PHE
                                        48.668 1.000 17.41
ANISOU 1805 CD2 PHE
                     264 1835
                                2359
                                             -440 433 112
                                        2419
                              15.247
       1806 CE1 PHE
                     264 5.661
                                       50.053 1.000 20.59
ATOM
ANISOU 1806 CE1 PHE
                     264 2616
                                2710
                                        2496
                                             -556 -425 7 2 5
                     264 3.458 16.133 49.906 1.000 22.51
       1807 CE2 PHE
ATOM
ANISOU 1807 CE2 PHE
                     264 2151
                                4047
                                        2355 -787 106 553
       1808 CZ
               PHE
                     264 4.386
                                15.350 50.562 1.000 20.88
ATOM
                     264 2889
265 7.676
ANISOU 1808 CZ
                                2376
                PHE
                                        2669 -936 -22 3 0 6
       1809 N
                                18.756
                                        44.811 1.000 11.81
MOTA
                LEU
                     265 1192
ANISOU 1809 N
                                                     47 1 9
                LEU
                                1248
                                        2047 -37
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                     265 7.900
ATOM
       1810 CA LEU
                                        2028 -223 16 - 63
ANISOU 1810 CA LEU
                     265 1264
                                1269
                                        42.703 1.000 12.10
ATOM
       1811 C
                LEU
                     265 7.915
                                17.617
ANISOU 1811 C
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                                        2033
                LEU
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ATOM
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                LEU
                LEU 265 1367
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ANISOU 1813 CB LEU 265 1399 1364
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ATOM
ANISOU 1814 CG LEU 265 1168 1399 2066 -292 -248 3
ATOM 1815 CD1 LEU 265 8.620 21.314 41.318 1.000 13.29
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ANISOU 1815 CD1 LEU
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MOTA
       1816 CD2 LEU
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ANISOU 1816 CD2 LEU
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ANISOU 1818 CA ARG
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 MOTA
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 MOTA
        1821 CB ARG
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 ANISOU 1821 CB ARG
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                                1477
       1822 CG ARG
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 MOTA
                                 1686 2207 -159 66 -115
15.041 43.993 1.000 12.70
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                ARG
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 MOTA
        1823 CD
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266 2.581
266 1343
266 1.304
 ANISOU 1823 CD
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                                               66 -22 8 4
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        1824 NE
                ARG
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                                 15.281 43.500 1.000 11.34
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                     266 1432
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 ANISOU 1825 CZ ARG
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 MOTA
                                               -11 -38 7 2
 ANISOU 1826 NH1 ARG
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 MOTA
        1827 NH2 ARG
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 ANISOU 1827 NH2 ARG
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                                                125
                     267 7.237
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                                 1394
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                                                16 -146 108
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                                                167
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 ANISOU 1830 C
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PRO 267 4.998
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                                           2164
       1832 CB PRO 267 8.238 13.761
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PRO 267 7.872
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ANISOU 1835 N
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ANISOU 1836 CA ASN
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ANISOU 1837 C
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ANISOU 1839 CB ASN
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       1840 CG ASN
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ANISOU 1840 CG ASN
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                     268 4.069
MOTA
       1841 OD1 ASN
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ATOM 1841 OD1 ASN 268 4.069
ANISOU 1841 OD1 ASN 268 2573
ATOM 1842 ND2 ASN 268 6.066
ANISOU 1842 ND2 ASN 268 2408
ATOM 1843 N ALA 269 3.531
ANISOU 1844 CA ALA 269 1677
ATOM 1844 CA ALA 269 3.278
ANISOU 1844 CA ALA 269 1459
ATOM 1845 C ALA 269 4.182
ANISOU 1845 C ALA 269 1289
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17.503 33.319 1.000 16.61
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12.712 34.594 1.000 13.99
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                                   1467
                                           2172
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ALA 269 4.581
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        1847 CB ALA 269 1.806
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ANISOU 1847 CB ALA 269 1300
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ASP 270 1688
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ANISOU 1849 CA ASP 270 1747
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270 6.749
270 1714
270 7.483
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                                                  -99
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                 ASP
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                                            2357
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                                                         139 226
                 ASP
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                                                   -80
                                   2354
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 ANISOU 1852 CB ASP
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                                                 -75
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                      270 5.386
 ATOM
        1854 OD1 ASP
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 ANISOU 1854 OD1 ASP
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 MOTA
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                 PHE
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        1857 CA PHE
 ATOM
 ANISOU 1857 CA PHE
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271 9.275 10.349
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10.349 32.325 1.000 13.31
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 MOTA
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                                                          28 2 1 8
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 MOTA
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 ANISOU 1859 O
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 ANISOU 1860 CB PHE
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        1861 CG PHE 271 10.386 11.791 34.516 1.000 14.56
 ATOM
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		- /4 -	
ANISOU 1861 CG PHE	271 1729 1	1320	2485 -152 34 -124
ATOM 1862 CD1 PHE	271 11.460 1	12.369	33.814 1.000 17.76
ANISOU 1862 CD1 PHE	271 1714 1	1581	3452 -235 393 -249
ATOM 1863 CD2 PHE	271 10.698 1	10.972	35.570 1.000 18.04
ANISOU 1863 CD2 PHE		1543	3130 -95 -540 1 7 2
ATOM 1864 CE1 PHE		12.092	34.166 1.000 17.54
ANISOU 1864 CE1 PHE	271 1838	1700	3128 -291 114 -50
ATOM 1865 CE2 PHE		10.609	35.899 1.000 18.84
ANISOU 1865 CE2 PHE		1646	3578 -392 -396 4 2 5
ATOM 1866 CZ PHE		11.154	35.162 1.000 17.25
ANISOU 1866 CZ PHE		1697	2415 -486 -19 -394
ATOM 1867 N THR		10.298	31.453 1.000 13.78
ANISOU 1867 N THR		1641	2083 30 19 1 5 4
ATOM 1868 CA THR		9.046	30.938 1.000 13.99
ANISOU 1868 CA THR		1660	2105 -99 83 6 7
ATOM 1869 C THR ANISOU 1869 C THR		8.841	31.410 1.000 14.71
ANISOU 1869 C THR ATOM 1870 O THR		1549 9.808	2441 -3 108 3 5 7 31.424 1.000 16.23
ANISOU 1870 O THR		1742	2780 -246 5 185
ATOM 1871 CB THR		9.117	29.388 1.000 16.27
ANISOU 1871 CB THR		2205	2119 191 125 8
ATOM 1872 OG1 THR		9.221	29.032 1.000 17.99
ANISOU 1872 OG1 THR		2473	2368 64 -190 264
ATOM 1873 CG2 THR		7.856	28.723 1.000 17.94
ANISOU 1873 CG2 THR		2167	
ATOM 1874 N PHE		7.600	31.743 1.000 14.91
ANISOU 1874 N PHE		1521	2499 92 238 2 1 8
ATOM 1875 CA PHE	273 13.894	7.253	32.254 1.000 15.16
ANISOU 1875 CA PHE	273 1602	1813	2345 296 277 5 5
ATOM 1876 C PHE	273 14.350	5.899	31.724 1.000 14.69
ANISOU 1876 C PHE		1647	2528 24 479 1 7 8
ATOM 1877 O PHE		5.086	31.262 1.000 15.91
ANISOU 1877 O PHE		1767	2541 -115 450 119
ATOM 1878 CB PHE		7.301	33.769 1.000 15.77 2314 -344 286 123
ANISOU 1878 CB PHE ATOM 1879 CG PHE		1921 6.336	2314 -344 286 123 34.424 1.000 14.54
ANISOU 1879 CG PHE		1726	2410 -95 -11 195
ATOM 1880 CD1 PHE	273 11.601	6.743	34.655 1.000 16.64
ANISOU 1880 CD1 PHE		2343	2521 -24 308 362
ATOM 1881 CD2 PHE	273 13.295	5.038	34.721 1.000 15.23
ANISOU 1881 CD2 PHE	273 1863	1624	2300 -110 91 1 3 6
ATOM 1882 CE1 PHE	273 10.719	5.848	35.259 1.000 16.10
ANISOU 1882 CE1 PHE	273 1593	2158	2365 -162 292 122
ATOM 1883 CE2 PHE	273 12.419	4.148	35.354 1.000 16.01
ANISOU 1883 CE2 PHE	273 1904	1980	2198 -139 285 181
ATOM 1884 CZ PHE	273 11.109	4.559	35.548 1.000 15.18
ANISOU 1884 CZ PHE	273 1843	2001	1925 -141 73 -227
ATOM 1885 N SER	274 15.634	5.612	31.926 1.000 15.31
ANISOU 1885 N SER ATOM 1886 CA SER	274 1559	1940	2317 361 383 247 31.518 1.000 15.37
ATOM 1886 CA SER ANISOU 1886 CA SER	274 16.221 274 1476	4.318 1723	2642 32 557 1 5 6
ATOM 1887 C SER	274 1476	3.284	32.588 1.000 14.67
ANISOU 1887 C SER	274 13.933		726 -113 265 3 0 2
ATOM 1888 O SER	274 16.310	3.476	33.770 1.000 15.98
ANISOU 1888 O SER	274 1668	1677	2728 126 143 193
ATOM 1889 CB SER	274 17.742	4.556	31.356 1.000 17.41
ANISOU 1889 CB SER	274 1487	2019	3112 235 945 725
ATOM 1890 OG SER	274 18.362	3.280	31.334 1.000 18.03
ANISOU 1890 OG SER	274 1839	1961	3052 293 840 188
ATOM 1891 N VAL	275 15.395	2.133	32.182 1.000 15.58
ANISOU 1891 N VAL	275 1646	1857	2417 -182 461 261

	- 75 -	
ATOM 1892 CA VAL		33.137 1.000 15.65
ANISOU 1892 CA VAL		2466 -180 261 265
ATOM 1893 C VAL		33.659 1.000 15.33
ANISOU 1893 C VAL ATOM 1894 O VAL		2139 116 392 - 45
ATOM 1894 O VAL ANISOU 1894 O VAL		34.871 1.000 15.68 2267 6 297 1 9 6
ATOM 1895 CB VAL		32.483 1.000 16.05
ANISOU 1895 CB VAL		2755 -76 405 2 1
ATOM 1896 CG1 VAL	2 275 14.080 -1.186	33.426 1.000 17.04
ANISOU 1896 CG1 VAI	275 2045 1688	2740 -211 230 1 5
ATOM 1897 CG2 VAL	275 12.847 0.608	32.203 1.000 18.45
ANISOU 1897 CG2 VAL ATOM 1898 N PRO		2928 -57 135 2 6 9 32.844 1.000 16.21
ANISOU 1898 N PRO		2532 97 589 3 6
ATOM 1899 CA PRO		33.399 1.000 18.10
ANISOU 1899 CA PRO	276 1736 2115	3025 147 616 - 93
ATOM 1900 C PRO		34.321 1.000 17.52
ANISOU 1900 C PRO		2697 97 469 2 3 9
ATOM 1901 O PRO ANISOU 1901 O PRO		35.348 1.000 19.66 3047 24 280 4 6 8
ATOM 1902 CB PRO	0 276 2013 2409	32.214 1.000 20.80
ANISOU 1902 CB PRO		3121 306 771 -249
ATOM 1903 CG PRO		30.999 1.000 21.57
ANISOU 1903 CG PRO		3046 340 802 -288
ATOM 1904 CD PRO ANISOU 1904 CD PRO		31.368 1.000 18.17 2546 179 832 -318
ATOM 1905 N LEG		34.027 1.000 17.09
ANISOU 1905 N LEU		3025 230 511 1 0 7
ATOM 1906 CA LEG		34.940 1.000 19.34
ANISOU 1906 CA LEU		3171 -219 218 2 6 2
ATOM 1907 C LET ANISOU 1907 C LET		36.249 1.000 18.34 3049 -33 -3 - 38
ATOM 1908 O LEG		37.319 1.000 19.29
ANISOU 1908 O LEG		3154 -271 -188 - 2
ATOM 1909 CB LET		34.291 1.000 21.41
ANISOU 1909 CB LET		3383 14 12 2 8 7
ATOM 1910 CG LET ANISOU 1910 CG LET		35.111 1.000 26.34 3978 -980 -547 9 4 4
ATOM 1911 CD1 LET		35.069 1.000 38.04
ANISOU 1911 CD1 LET	U 277 3764 3171	7518 -487 -2057 853
ATOM 1912 CD2 LET		34.631 1.000 31.98
ANISOU 1912 CD2 LET		6109 -366 508 732
ATOM 1913 N ALI ANISOU 1913 N ALI		36.202 1.000 17.30 2793 74 218 1 1 5
ATOM 1914 CA AL		37.464 1.000 16.75
ANISOU 1914 CA AL	A 278 2200 1566	2600 216 146 - 2
ATOM 1915 C AL.		38.313 1.000 16.31
ANISOU 1915 C AL.		2794 -337 -196 1 0 7
ATOM 1916 O AL. ANISOU 1916 O AL.		39.523 1.000 17.26 2754 -62 -53 2 0 5
ATOM 1917 CB AL		37.177 1.000 17.55
ANISOU 1917 CB AL	A 278 2109 1880	2679 295 195 - 11
ATOM 1918 N AR		37.696 1.000 17.07
ANISOU 1918 N AR ATOM 1919 CA AR		2766 -178 26 3 0 8
ATOM 1919 CA AR ANISOU 1919 CA AR		38.473 1.000 16.93 2323 15 -241 203
ATOM 1920 C AR		39.098 1.000 19.87
ANISOU 1920 C AR	G 279 2491 2292	2766 -487 -384 5 4 3
ATOM 1921 O AR		40.234 1.000 33.04
ANISOU 1921 O AR ATOM 1922 CB AR		4115 -1726 -1700 2603
ATOM 1922 CB AR	G 2/3 10.104 -2.U42	37.517 1.000 20.04

									1 (1/32)0/00000
ANISOU	1922	СЪ	A D C	270	2040	- 76 -			
ATOM	1923		ARG ARG	279 2	2042 16.742	1609	3964		-221 - 305
ANISOU			ARG	279 2		-2.491 2728			
ATOM	1924		ARG		16.601	-3.422			-401 - 351 24.81
ANISOU			ARG	279 3		2982	3231		24.81 07 -609
ATOM	1925	ΝE	ARG		17.575	-4.484	36 195	1 000	27.50
ANISOU			ARG	279 4		2656	3463	355	-146 - 181
ATOM	1926		ARG		17.301	-5.725	36.620		41.33
ANISOU			ARG	279 7		2466	5519	-186	
ATOM	1927	NHI	ARG	279 1	16.024	-6.012	36.866		40.58
ANISOU ATOM	1927	NHI	ARG	279 8		3012	3585		507 452
		NHZ	ARG	279 9	L8.200	-6.688	36.807		
ATOM	1929		GLU		20.390	2227 0.119	8496	-127	-4607 - 463
ANISOU			GLU	280 2		2276	38.424 3028		
ATOM	1930		GLU		21.748	0.334	38.948	84 324	1 1 2 b
ANISOU	1930		GLU	280 2		2274	3385	25 581	
MOTA	1931		GLU		21.705	1.257	40.182	1.000	20.67
			GLU	280 2		1968	3552	-281	285 2 0
ATOM ANISOU	1932		GLU		22.723	1.079	40.908		26.81
ANISOU	1932		GLU GLU	280 2	2659	3419	4107		-183 - 87
ANISOU			GLU	280 2	22.651	1.029 2558	37.926		
ATOM	1934		GLU		22.997	0.342	4044 36.634	-351	1022 3 0 3
ANISOU			GLU	280 2	2605	4888	2816	596	116 623
MOTA	1935	CD	GLU	280 2	23.815	1.298	35.760		
ANISOU			GLU	280 4		7780	3903	-1328	1206 8 3 4
ATOM ANISOU	1936	OE1	GLU		24.541	2.171	36.296	1.000	41.36
ATOM	1936	OET	GLU	280 2		6033	7015	27 109	99690
ANISOU	1937	OE2	GLU		23.727	1.219	34.520	1.000	64.81
ATOM	1938	N	CYS		20.777	10028 2.156	3751 40.313	1 000	1104 2134
ANISOU	1938	N	CYS	281 2		2240	3599	-211	532 - 238
ATOM	1939	CA	CYS	281 2	0.481	3.164	41.337		24.33
ANISOU			CYS	281 2		2911	4219	-526	1121 - 817
ATOM ANISOU	1940	C	CYS		9.858	2.568	42.585		
ATOM	1941		CYS CYS	281 2	.492 .9.789	3261	4546	-1608	1457 - 1343
ANISOU			CYS	281 1		3.161 2012	43.685		
ATOM	1942		CYS		.9.632	4.438	3282 40.795	-250	-326 1 3 5
ANISOU			CYS	281 1		3088	4063	-286	100 -2108
ATOM	1943						39.444		
ANISOU			CYS	281 1	.0822	4742	4730	-3261	1316 4 5
ATOM ANISOU	1944	N	GLY	282 1	.9.370	1.317	42.565	1.000	18.81
ATOM	1944		GLY GLY	282 1		2224	3695		19 - 206
ANISOU	1945	CA	GLY	282 1	8.675	0.750 1771	43.744		
ATOM	1946		GLY		.7.194		3171 43.538		52 -168
ANISOU	1946	C	GLY	282 1		1645	2417		-453 3 7 8
ATOM	1947	0	GLY	282 1	6.480		44.380		
ANISOU			GLY	282 1		1921	2306	-211	-399 3 6 0
ATOM	1948	N	PHE	283 1	.6.625	0.919	42.404		
ANISOU ATOM	1948		PHE	283 1		1539	2006		-336 - 115
ANISOU	1949	CA	PHE PHE	283 1	.5.173	0.829 1410	42.203		
ATOM	1950		PHE		.4.810	-0.604	2428 41.809		-670 4 6
ANISOU	1950	С	PHE	283 1	519	1314	2137		-338 1 7 4
ATOM	1951	0	PHE	283 1	.5.311	-1.184	40.837	1.000	
ANISOU			PHE	283 1	366	1418	2578	-142	-78 1 7
ATOM ANISOU	1952	CB	PHE	283 1	4.749	1.800	41.078		13.76
MT200	1332	CB	PHE	283 1	814	1288	2125	-39	-268 0

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41.512 1.000 14.75
                    283 14.842 3.269
ATOM
       1953 CG PHE
ANISOU 1953 CG PHE
                    283 1985
                               1363
                                      2255
                                             12 -317 -
       1954 CD1 PHE
                    283 13.814 3.904
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ANISOU 1954 CD1 PHE
                    283 2318
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                                              303
                    283 15.994 3.999
                                       41.298 1.000 17.72
       1955 CD2 PHE
ATOM
ANISOU 1955 CD2 PHE
                    283 2526
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                                            -307 -89 272
                                      42.655 1.000 20.78
       1956 CE1 PHE
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 ANISOU 1981 CA LEU
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 ANISOU 1982 C
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        1983 0
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	0.00					- 78 -			
ANISOU 1			LEU	287		2275	2645		300 - 275
	.984		LEU		9.954	-1.480			
ANISOU 1			LEU		1773	1380	2306		248 107
	1985		LEU		9.362	-0.603	35.231		
ANISOU 1			LEU	287		1496	2523	62 52	
	1986				10.143	0.705	35.413		
ANISOU 1				287		1444	2403	0 -14	
	1987				7.921	-0.197			
ANISOU 1					1476	2035	2579		-100 - 7
	1988		ASP		9.256	-4.060	31.958		
ANISOU 1			ASP		2041	1611	2081	73 175	
	1989		ASP		9.764	-4.722	30.757		
ANISOU 1			ASP	288		2028	2268		314
	1990		ASP		10.437	-3.682	29.874		
ANISOU 1			ASP		2484	2597	2040		97 8 1
ATOM 1 ANISOU 1	1991		ASP	288	9.998 3382	-2.526			
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ATOM 3			ASP		8.659 2431	-5.490 2414	30.060 2460		258 - 720
	1993		ASP		9.139	-6.468	29.000		
ANISOU 3			ASP		2688	2223	2499		393 - 552
	1994				10.173	-7.145	29.185		
ANISOU					3134	3038	4100		427 - 716
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ANISOU					3596	4859	3325	307	-361 -2100
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ANISOU			GLY		2960	2893	2765		778 116
	1997		GLY		12.008	-3.083	28.169		
ANISOU :			GLY		3678	3562	2486		
	1998		GLY		12.988	-2.078	28.725		
ANISOU :	1998	С	GLY		2567	2916	2528	-485	353 150
MOTA	1999	0	GLY	289	13.411	-2.097	29.891	1.000	23.72
ANISOU :	1999	0	GLY	289	3428	3219	2364	-1104	440 113
ATOM :	2000	N	GLU	290	13.402	-1.168	27.818		
ANISOU :	2000	N	GLU		2246	2396	2319	-145	616 -115
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ANISOU :			GLU		1912	2419			0 - 3 6 7
	2002		GLU		14.261	1.058			17.90
ANISOU			GLU		2180	2308	2313		1 - 2 9 7
	2003		GLU		15.143	1.619			17.58
ANISOU			GLU		2525	2050	2104	-35	380 165
	2004	_	GLU		15.341	-0.161			23.21
ANISOU			GLU		3184	2508	3126	-273	1753 - 467
	2005		GLU		15.833	-1.492			24.55
ANISOU ATOM	2005		GLU		3609	2992	2725	348	1232 - 743 30.03
ANISOU			GLU GLU		16.676 3365	-2.280 3708	4337	476	753 - 211
	2007				17.492	-1.684			40.04
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			GLU		16.622	-3.527	27 237		51.76
ANISOU					8785	3812	7070	-12	-483 1583
	2009		THR		13.064	1.578			18.14
ANISOU			THR		2305	2486	2103	224	711 - 321
	2010		THR		12.697	2.896	29.049		18.72
	2010		THR		2521	2080	2511	105	1131 6 6
	2011		THR		11.278	2.744			15.79
ANISOU	2011	. C	THR		2178	1758	2064	134	538 - 50
ATOM	2012		THR		10.517	1.834	29.217		18.62
ANISOU			THR		2764	1966	2344	-248	664 - 311
MOTA	2013		THR		12.722	4.031			21.54
ANISOU	2013	CB	THR	291	3043	2625	2516	-164	891 362

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						- 13 -		
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ANISOU					3160	4072	2641	-86 703 503
ATOM ANISOU	2015	CG2	THR		14.048	4.115	27.292	1.000 24.20
ATOM	2015				3199	3832	2164	-445 930 533
ANISOU			ALA ALA	292	10.959	3.658	30.492	
ATOM	2017		ALA	292	1637	1656	2347	200 429 -153
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ATOM	2018		ALA		9.356	1477 5.065	2294	170 299 7 8
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ATOM	2019		ALA	292	10.228	5.939	31 710	60 144 - 139 1.000 14.27
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ATOM	2020	CB	ALA		9.670	2.754		1.000 14.02
ANISOU			ALA	292		1580	2053	37 22 - 27
ATOM	2021		THR	293	8.054	5.258		1.000 13.54
ANISOU			THR	293	1468	1617	2058	117 373 -118
ATOM	2022		THR		7.605	6.546		1.000 13.40
ANISOU			THR	293	1565	1647	1877	152 209 -232
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ATOM	2026				5.273	6.112		95 345 3 4 5 1.000 13.75
ANISOU	2026	OG1	THR	293	1672	1570	1981	-12 314 135
ATOM	2027	CG2	THR		6.476	7.139		1.000 15.93
ANISOU			THR	293	2121	2022	1911	255 434 3 3 7
MOTA	2028		PHE		7.241	7.661		1.000 12.81
ANISOU			PHE		1607	1440	1822	-83 149 -151
ATOM	2029		PHE		6.857	7.773		1.000 12.37
ANISOU ATOM			PHE		1332	1469	1899	-267 166 -289
ANISOU	2030		PHE		5.556	7.022		1.000 12.36
ATOM	2030		PHE PHE		1336 5.403	1361	1999	-151 30 - 36
ANISOU			PHE		1556	6.253 1410		1.000 13.27
ATOM	2032		PHE		6.698	9.271	2076 36.267	-191 183 4 6
ANISOU			PHE	294	2039	1351	1866	1.000 13.83 -192 -29 -177
ATOM	2033	CG	PHE	294	6.306	9.488		1.000 13.10
ANISOU			PHE		1786	1216	1974	-125 -63 -244
MOTA	2034	CD1	PHE	294	7.207	9.411		1.000 17.41
ANISOU					2132	2533	1952	-1012 -287 7 6
ATOM	2035	CD2	PHE		4.964	9.739	38.026	1.000 18.41
ANISOU ATOM	2035	CD2	PHE		2156	2263	2575	565 332 5 7
ANISOU	2036	CEL	PHE		6.810	9.608		1.000 17.72
ATOM	2037	CES	DHE		2348	2296	2086	-308 -362 -136
ANISOU	2037	CE2	DHE		4.591 2078	10.010		1.000 19.37
ATOM	2038		PHE		5.507	2541 9.956	2740	330 232 -630
ANISOU			PHE		2443	1678	2855	1.000 18.36 -394 -55 -245
ATOM	2039	N	GLN		4.588	7.205		1.000 12.59
ANISOU	2039	N	GLN		1248	1429	2106	-62 38 - 168
ATOM	2040	CA	GLN	295	3.320	6.484		1.000 12.76
ANISOU			GLN	295	1266	1215	2365	7 -157 -117
ATOM	2041	C	GLN		3.512	4.984	35.318	
ANISOU			GLN	295	1449	1256	1944	10 1 - 7 3
ATOM ANISOU	2042		GLN		2.922	4.238		1.000 13.61
ATOM	2042		GLN	295	1323	1427	2424	7 85 1 5 5
ANISOU	2043	CB	GLN GLN	4 7 3 2 0 E	2.375 1227	6.975	34.317	
ATOM	2044		GLN	295		1594 6.256	2616	81 -133 192 1.000 14.03
						0.200	34.249	1.000 14.03

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ANISOU 2045 CD ATOM 2046 OE1 ANISOU 2047 NE2 ANISOU 2048 N ANISOU 2049 CA ANISOU 2050 C ANISOU 2051 O ANISOU 2051 O ANISOU 2055 OD2 ANISOU 2055 OD2 ANISOU 2056 N ANISOU 2056 N ANISOU 2057 CA ANISOU 2056 N ANISOU 2057 CA ANISOU 2056 N ANISOU 2057 CA ANISOU 2057 CA ANISOU 2058 C ANISOU 2058 C ANISOU 2058 C ANISOU 2058 C ANISOU 2059 O ANISOU 2059 O ANISOU 2060 CB ANI	GLN 295 0.157 GLN 295 1305 GLN 295 0.459 GLN 295 0.459 GLN 295 1811 GLN 295 -0.982 GLN 295 1225 ASP 296 4.363 ASP 296 1425 ASP 296 1628 ASP 296 1628 ASP 296 1534 ASP 296 1534 ASP 296 1534 ASP 296 5.709 ASP 296 1655 ASP 296 6.212 ASP 296 6.212 ASP 296 6.212 ASP 296 1655 ASP 296 1655 ASP 296 1655 ASP 297 1325 TRP 297 6.038 TRP 297 1325 TRP 297 1554 TRP 297 1130 TRP 297 1130 TRP 297 1130 TRP 297 1130 TRP 297 1143 TRP 297 1554 TRP 297 1615 TRP 297 1615 TRP 297 1615 TRP 297 1327 TRP 297 1615 TRP 297 1327 TRP 297 1615 TRP 297 10.318 TRP 297 10.318 TRP 297 10.318 TRP 297 2916 TRP 297 2916 TRP 297 10.258	1486 7.6516 19.4663 13.07469 13.07469 13.074683 13.074683 13.60048 13.074683 13.60048 13.60048 15.7359 14.990 15.0803 16.1833 16.1833 16.393 1	2493
ATOM 2069 CH2	TRP 297 10.258	5.546	42.397 1.000 23.53
ANISOU 2069 CH2	TRP 297 3298	2356	3285 -320 -1146 -344
ATOM 2070 N	ILE 298 5.106	4.167	39.044 1.000 13.58
ANISOU 2070 N	ILE 298 1324	1726	2108 241 -167 1 2 7
ANISOU 2071 CA	ILE 298 1413	2177	1986 -13 -161 -208
ATOM 2072 C	ILE 298 2.841	4.054	40.121 1.000 12.02
ANISOU 2072 C	ILE 298 1455	1300	1813 56 -239 402
ATOM 2073 O	ILE 298 2.182	3.782	41.147 1.000 13.67
ANISOU 2073 O	ILE 298 1732	1582	1881 -23 -4 193
ATOM 2074 CB	ILE 298 4.428	5.914	40.673 1.000 19.45
ANISOU 2074 CB	ILE 298 2261	2446	2683 -699 237 -835

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ATOM	2075	CG1	ILE	298 5.907	6.245	41.001	1.000	27.83
ANISOU				298 2776	4275	3525	-1314	-556 -1030
MOTA	2076			298 3.679	6.319	41.929		
ANISOU				298 3770	3344		-57	255 - 983
ATOM	2077			298 6.368	5.628	42.306		
ANISOU				298 4561	7224		-652	
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ATOM	2078		GLY	299 2.317		38.893		
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ATOM	2079		GLY	299 0.918	3.741	38.670		
ANISOU			GLY	299 1276	1279		106	-188 -154
ATOM	2080		GLY	299 0.135	5.017	38.378		
ANISOU			GLY	299 1421	1403		113	-231 1 1 8
ATOM	2081		GLY	299 0.738	6.025	38.017		
ANISOU			${ t GLY}$	299 1713	1353	2252	122	289 - 13
ATOM	2082	\mathbf{N}	GLY	300 -1.183	4.917	38.447	1.000	13.08
ANISOU	2082	N	GLY	300 1325	1545		146	-267 -145
ATOM	2083	CA	GLY	300 -2.075	5.966	37.992	1.000	
ANISOU	2083	CA	GLY	300 1447	1521	2143	116	-415 -143
MOTA	2084	С	GLY	300 -2.519	6.972	39.042	1.000	12.94
ANISOU	2084	С	GLY	300 1098	1365	2456	-52	-407 -192
MOTA	2085		GLY	300 -3.262		38.672		13.39
ANISOU	2085	0	GLY	300 1321	1342		-19	-217 - 45
ATOM	2086		ASN	301 -1.973		40.254		
ANISOU			ASN	301 1494	1429		-225	
ATOM	2087		ASN	301 -2.162		41.313		
ANISOU			ASN	301 1590	1435		-194	-38 - 61
ATOM	2088		ASN	301 -0.837		41.885		
ANISOU			ASN	301 1676	1268	1791	-35	-142 - 20
ATOM	2089		ASN	301 -0.007		42.169		
ANISOU			ASN	301 1831	1355	2093	73 -1	
ATOM	2090		ASN	301 -3.075				16.01
ANISOU			ASN	301 1632	1909	2542		4 3 1 5
MOTA	2091		ASN	301 -3.942				18.23
ANISOU			ASN	301 1986	2508	2435	190	152 - 90
ATOM	2092			301 -4.973		42.614		
ANISOU				301 1606	1626	3394	-21	144 -190
ATOM			ASN	301 -3.518				33.30
ANISOU				301 2804	6923	2928	1012	
ATOM	2094		TYR	302 -0.595				12.96
ANISOU			TYR	302 1662	1278	1985	-69	-21 -135
ATOM	2095		TYR	302 0.674	9.948			13.48
ANISOU			TYR	302 0.074	1259	2192	-130	-132 3 4
ATOM	2096		TYR	302 0.768	9.269			12.63
ANISOU			TYR	302 0.788	1293	2092	53 44	
ATOM	2097		TYR	302 -0.218				14.15
ANISOU			TYR	302 1332	1737	2305	-65	48 - 27
ATOM	2098			302 0.764				13.30
			TYR		11.472			33 4 1
ANISOU ATOM			TYR	302 1635	1192	2226	-81) 12.02
ANISOU	2099		TYR	302 1.159	12.143			-25 - 271
			TYR	302 1586	1103	1880	-59 1 000	
ATOM			TYR	302 2.501	12.233			13.11
ANISOU			LTYR	302 1633	1284	2066	-80	11 - 18
ATOM			TYR	302 0.235	12.709			12.52
ANISOU				302 1576	1132	2049	-44	13 - 127
ATOM			LTYR	302 2.933	12.822	40.119		12.29
ANISOU			LTYR	302 1581	1043	2045	-185	-84 -77
ATOM			2 TYR		13.273			14.12
ANISOU					1443	2458	-241	15 3 2 5
ATOM		4 CZ	TYR		13.347			12.69
ANISOU			TYR		1224	2113	-287	-91 1 0
ATOM	210	5 OH	TYR	302 2.376	13.866	38.013	1.000	0 13.42

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				- 62 -		
ANISOU	2105 ОН	TYR	302 1505	1469	2124	-93 33 1 4 6
ATOM	2106 N	VAL	303 1.956			
	2106 N			8.855		1.000 13.92
		VAL	303 1406	1637	2246	153 88 9 9
ATOM	2107 CA	VAL	303 2.355	8.336	45.746	1.000 14.51
ANISOU	2107 CA	VAL	303 1838	1320	2355	-137 -391 - 74
ATOM	2108 C	VAL	303 3.498	9.244		1.000 15.23
	2108 C	VAL	303 1404	1507	40.239	1.000 15.23
				1507	2876	
ATOM	2109 0	VAL	303 4.471	9.386	45.512	1.000 18.70
ANISOU	2109 0	VAL	303 1859	1861	3386	-239 326 -504
ATOM	2110 CB	VAL	303 2.856	6.880		1.000 16.75
ANTSOU	2110 CB	VAL	303 2140	1319	2905	
ATOM	2111 CG1					16 -759 -123
	2111 CG1	VAL	303 3.279	6.401		1.000 19.53
	2111 CG1		303 2185	1951	3284	232 -1054 148
ATOM	2112 CG2		303 1.723	5.956	45.125	1.000 17.82
ANISOU	2112 CG2	VAL	303 2476	1442	2852	-213 -558 - 406
MOTA	2113 N	ASN	304 3.349	9.900		1 000 1 1 0 7
	2113 N	ASN	304 1409		47.378	
				1369	2566	-39 -407 - 86
ATOM	2114 CA	ASN	304 4.317	10.928	47.772	1.000 14.31
ANISOU	2114 CA	ASN	304 1474	1387	2578	-102 -424 - 55
ATOM	2115 C	ASN	304 5.450	10.397		1.000 13.75
ANISOU	2115 C	ASN	304 1360	1487	2378	34 -274 - 87
ATOM	2116 0	ASN	304 6.539	10.962	40 504	
	2116 0		204 0.339			1.000 14.60
		ASN	304 1314	1795	2438	-34 -55 -320
ATOM	2117 CB	ASN	304 3.589	12.035	48.551	1.000 14.26
	2117 CB	ASN	304 1710	1214	2494	6 -303 176
ATOM	2118 CG	ASN	304 2.535	12.661		1.000 14.81
ANISOU	2118 CG	ASN	304 1551	1627	2449	23 -114 4 0 2
ATOM	2119 OD1		304 2.866	13.255		
	2119 OD1	A CM				1.000 16.52
			304 1896	1746	2636	80 19 5 8 9
ATOM	2120 ND2	ASN	304 1.290	12.595	48.102	1.000 18.43
ANISOU	2120 ND2	ASN	304 1560	2980	2463	127 -10 199
ATOM	2121 N	ILE	305 5.175	9.413		1.000 16.36
ANISOU	2121 N	ILE	305 1546	1553	3117	-78 -503 2 6 6
ATOM	2122 CA	ILE	305 6.173	8.890		
	2122 CA	ILE		0.090	50.407	1.000 14.85
			305 1670	1537	2436	165 -277 - 40
ATOM	2123 C	ILE	305 6.183	7.372	50.352	1.000 15.78
	2123 C	ILE	305 1527	1555	2914	95 -438 - 51
ATOM	2124 0	ILE	305 5.231	6.736	49.886	1.000 17.54
ANISOU	2124 0	ILE	305 1463	1789	3412	
ATOM	2125 CB	ILE	305 5.949	9.430		1.000 17.80
	2125 CB	ILE	305 2167			
ATOM	2126 CG1			1962	2634	-23 265 -209
	2120 CG1	. TPE	305 4.578	9.091	52.416	1.000 18.93
ANISOU	2126 CG1	. ILE	305 1716		2526	1 -218 -163
MOTA	2127 CG2	ILE	305 6.171	10.944	51.823	1.000 19.17
ANISOU	2127 CG2	ILE	305 2685	1863	2737	70 -534 -405
ATOM	2128 CD1	ILE	305 4.415	9.459		1.000 21.28
	2128 CD1	TIF	305 2521	2902		
ATOM	2129 N				2662	19 452 - 71
	2123 N	ARG	306 7.246	6.806		1.000 14.59
	2129 N	ARG	306 1738	1641	2165	52 -356 271
ATOM	2130 CA	ARG	306 7.424	5.360	50.828	1.000 15.25
ANISOU	2130 CA	ARG	306 1509	1663	2622	139 -302 7 7
ATOM	2131 C	ARG	306 8.234	4.903		1.000 15.02
ANISOU	2131 C	ARG	306 1588	1464		
ATOM	2132 0				2656	133 -332 - 21
		ARG	306 9.141	5.614		1.000 16.63
	2132 0	ARG	306 1682	2101	2536	-219 -294 -168
ATOM	2133 CB	ARG	306 8.135	4.943	49.532	1.000 16.31
	2133 CB	ARG	306 1820	1681	2697	
MOTA	2134 CG	ARG	306 8.226	3.414		1.000 18.43
ANISOU	2134 CG	ARG	306 2476	1700	2828	40 -194 -156
ATOM	2135 CD	ARG	306 8.401			
	2135 CD			3.068		1.000 18.26
1111 7 2 0 0	2133 CD	ARG	306 2087	1971	2880	-120 -145 -330

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2136 NE ARG 306 7.136 3.228 47.188 1.000 20.53 ANISOU 2136 NE ARG 306 2442 2013 3345 -577 -668 -234 2137 CZ ARG 306 6.980 3.178 45.873 1.000 20.27 ATOM 2137 CZ ARG 306 5.980 3.178

ANISOU 2137 CZ ARG 306 2330 2057

ATOM 2138 NH1 ARG 306 8.086 3.000

ANISOU 2138 NH1 ARG 306 2136 2580

ATOM 2139 NH2 ARG 306 5.759 3.250

ANISOU 2139 NH2 ARG 306 2107 1838

ATOM 2140 N ARG 307 7.898 3.775

ANISOU 2140 N ARG 307 2716 1872

ATOM 2141 CA ARG 307 8 576 3 212 3316 373 -522 2 0 45.107 1.000 22.13 274 -589 - 723 3695 45.341 1.000 18.44 3062 259 -285 8 4 52.612 1.000 19.10 2671 -294 -607 3 2 7 307 8.576 3.212 53.768 1.000 21.13 307 3321 2201 2504 -48 -845 1 307 9.536 2.138 53.277 1.000 23.30 2141 CA ARG ATOM ANISOU 2141 CA ARG 2504 -48 -845 1 3 9 MOTA 2142 C ARG ANISOU 2142 C ARG 307 3417 2170 3267 181 -1046 3 9 ARG 307 9.385 2143 0 ATOM 52.187 1.000 21.01 1.601 ANISOU 2143 O ARG 307 2574 2355 3052 174 -728 1 1 2 307 7.557 2.522 307 4545 3184 2144 CB ARG MOTA 54.694 1.000 27.30 ANISOU 2144 CB ARG 2645 -13 -247 7 0 5 ATOM 2145 CG ARG 307 6.839 3.488 55.629 1.000 46.30 ANISOU 2145 CG ARG 307 6310 6374 4907 215 1655 - 970 ATOM 2146 CD ARG 307 7.054 3.085 57.085 1.000 66.50 ANISOU 2146 CD ARG 307 11107 10355 3806 -2980 2792 -1145 ATOM 2147 NE ARG 307 5.989 2.203 57.531 1.000 78.91 ANISOU 2147 NE ARG 307 11821 12833 5330 -4530 1969 -ATOM 2148 CZ ARG 307 5.987 1.285 ANISOU 2148 CZ ARG 307 7704 14382 58.479 1.000 73.67 5907 -4724 1249 1051 ATOM 2149 NH1 ARG 307 7.063 1.038 59.214 1.000 80.32 ANISOU 2149 NH1 ARG 307 6613 17949 5955 -3290 2179 1 0 5 ATOM 2150 NH2 ARG 307 4.872 0.597 58.707 1.000 73.74 ARG 307 9116 15919 2983 -6954 438 -917 THR 308 10.551 1 861 54 113 1000 73.74 ANISOU 2150 NH2 ARG ATOM 2151 N 308 10.551 1.861 54.113 1.000 25.61 ANISOU 2151 N THR 308 4234 2212 3285 536 -1421 -232 THR 308 11.308 0.640 53.822 1.000 30.02 THR 308 3468 1939 5998 225 -1629 THR 308 10.468 -0.611 54.030 1.000 25.42 ATOM 2152 CA THR 53.822 1.000 30.02 ANISOU 2152 CA THR 5998 225 -1629 -194 ATOM 2153 C THR 308 2915 2190 THR 308 9 523 -0.768 ANISOU 2153 C ATOM 2154 0 THR 308 9.523 3482 ANISOU 2154 O THR 308 4042 2155 CB THR 308 12.581 0.531 ATOM 54.688 1.000 26.09 ANISOU 2155 CB THR 308 2701 3586 3626 242 -361 - 456 2156 OG1 THR 308 12.140 0.751 ATOM 56.028 1.000 32.90 ANISOU 2156 OG1 THR 308 4146 4188 ATOM 2157 CG2 THR 308 13.577 1.594 4167 504 745 - 495 54.256 1.000 31.43 ANISOU 2157 CG2 THR 308 3193 4702 4047 -577 -132 -538 ATOM 2158 N SER 309 10.850 -1.591 53.217 1.000 24.73 ANISOU 2158 N SER 309 2934 2092 4370 94 -574 -391 2159 CA SER 309 10.199 -2.897 53.230 1.000 25.19 ATOM ANISOU 2159 CA SER 309 3793 2464 3316 -485 451 -230 MOTA 2160 C SER 309 10.466 -3.691 54.512 1.000 24.06 ANISOU 2160 C SER 309 2360 2888 3893 302 107 3 5 ATOM 2161 0 SER 309 11.565 -3.621 55.084 1.000 34.54 SER 309 3626 2131 7366 -76 -1944
SER 309 10.639 -3.700 52.012 1.000 26.52
SER 309 3970 2159 3948 167 580 SER 309 10.217 -5.039 52.148 1.000 26.34
SER 309 3198 2207 4604 156 -844 -ANISOU 2161 0 -1944 - 34ATOM 2162 CB ANISOU 2162 CB 580 - 366 ATOM 2163 OG ANISOU 2163 OG SER 309 3198 2207 4604 156 -844 - 260 ATOM 2164 N LYS 310 9.494 -4.458 54.961 1.000 24.99 ANISOU 2164 N LYS 310 3172 2459 3864 160 262 366 ATOM 2165 CA LYS 310 9.651 -5.339 56.125 1.000 28.38 ANISOU 2165 CA LYS 278 281 ATOM 2166 C LYS 310 9.941

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ANISOU 2166 C
                LYS
                     310 3371
                                 2687
                                         3846
                                                168
                                                      -290 5 7 7
MOTA
       2167 0
                LYS
                     310 10.150
                                -7.684 56.515 1.000 33.48
ANISOU 2167 O
                LYS
                     310 5267
                                 3056
                                         4400
                                                -66
                                                      -450 1073
MOTA
       2168 CB
                     310 8.299
               LYS
                                 -5.367
                                         56.858 1.000 37.77
ANISOU 2168 CB LYS
                     310 5736
                                 4695
                                         3921
                                                299
                                                      1818 1 8
ATOM
       2169 CG
               LYS
                     310 8.014
                                 -4.214
                                         57.806 1.000 40.55
ANISOU 2169 CG
               LYS
                     310 6395
                                 4716
                                         4295
                                                1525
                                                      1524 1 0 1
ATOM
       2170 CD LYS
                     310 6.798
                                 -4.587
                                         58.649 1.000 44.24
ANISOU 2170 CD
               LYS
                     310 9091
                                 4224
                                         3495
                                                1053
                                                      2816 5 8 4
MOTA
       2171 CE
               LYS
                     310 6.722
                                 -6.109 58.818 1.000 59.12
ANISOU 2171 CE
               LYS
                     310 9281
                                 4577
                                         8606
                                                766
                                                      -82 2478
ATOM
       2172 NZ
                     310 6.088
               LYS
                                -6.563
                                        60.089 1.000 55.80
ANISOU 2172 NZ
               LYS
                     310 4884
                                 5742
                                         10577 287
                                                     -947 4796
ATOM
       2173 N
                ALA
                     311 9.896
                                 -7.030
                                        54.410 1.000 22.45
ANISOU 2173 N
                ALA
                     311 2190
                                 2402
                                         3939
                                                10 52 2 6 9
ATOM
       2174 CA
                     311 10.360 -8.369 53.972 1.000 31.89
               ALA
ANISOU 2174 CA
               ALA
                     311 3771
                                 2594
                                         5753
                                                434
                                                      -516 - 421
MOTA
       2175 C
                     311 11.909
                ALA
                                -8.459
                                        53.833 1.000 23.30
ANISOU 2175 C
                ALA
                     311 3907
                                 2328
                                         2616
                                                1393 -593 1 1 2
ATOM
       2176 CB
               ALA
                     311 9.619
                                 -8.665 52.674 1.000 27.94
ANISOU 2176 CB
               ALA
                     311 2407
                                 2878
                                         5329 -355 542 -672
       2177 OW
ATOM
                     501 -6.477
               HOH
                                10.237
16.189
                                        44.256 1.000 15.66
       2178 OW HOH
ATOM
                     502 -9.349
                                        51.010 1.000 19.26
       2179 OW HOH
ATOM
                     503 -1.489 3.653
                                         34.560 1.000 15.78
MOTA
       2180 OW HOH
                     504 -10.499 18.731
                                         50.182 1.000 16.19
ATOM
       2181 OW HOH
                     505 -8.612 16.958
                                        47.640 1.000 17.30
42.881 1.000 19.05
ATOM
       2182 OW HOH
                     506 -10.255 20.839
ATOM
       2183 OW HOH
                    507 2.096
                                 1.076
                                         32.810 1.000 29.32
MOTA
       2184 OW HOH
                    508 -0.284 4.743
                                         41.885 1.000 13.93
       2185 OW HOH
ATOM
                    509 -8.525 18.553 42.416 1.000 21.33
       2186 OW HOH
ATOM
                    510 3.165
                                         43.488 1.000 24.59
                                 2.604
       2187 OW HOH 511 -6.282 19.386 52.341 1.000 18.98
ATOM
ATOM
       2188 OW HOH 512 -6.826 24.638
                                        46.833 1.000 21.77
       2189 OW
ATOM
               HOH
                    513 10.510 -4.344
                                        46.092 1.000 25.88
ATOM
       2190 OW
               HOH 514 -0.806 16.964
                                        40.372 1.000 16.54
ATOM
                    515 -1.269 18.855
       2191 OW
               нон
                                        42.411 1.000 15.76
ATOM
       2192 OW
               HOH
                     516 14.277
                                -5.146
                                        40.175 1.000 15.53
ATOM
       2193 OW
                     517 -0.123 21.538
                HOH
                                        40.640 1.000 17.22
ATOM
       2194 OW
                HOH
                     518 13.131
                                -0.967
                                        51.791 1.000 31.17
ATOM
       2195 OW
                     519 11.009 2.875
                HOH
                                         45.599 1.000 20.20
ATOM
       2196 OW
                HOH
                     520 5.789
                                13.543
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ATOM
       2197 OW
                HOH
                     521 2.168
                                 19.767
                                        55.925 1.000 20.41
ATOM
       2198 OW
                     522 8.487
                HOH
                                 15.960 34.949 1.000 15.40
MOTA
       2199 OW
               HOH
                     523 10.794
                                12.697
                                        29.921 1.000 19.99
ATOM
       2200 OW
                     524 -11.722 19.112
               HOH
                                        44.516 1.000 19.82
ATOM
       2201 OW
                     525 1.672
               HOH
                                -2.081
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       2202 OW
ATOM
               HOH
                     526 9.651
                                 15.283
                                         32.342 1.000 20.37
ATOM
       2203 OW
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               HOH
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32.041 1.000 19.60
                                31.187
ATOM
       2204 OW
               HOH
                     528 15.326
                                 11.252
ATOM
       2205 OW
               HOH
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                                 26.984
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MOTA
       2206 OW
               HOH
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                                         50.915 1.000 16.17
52.682 1.000 19.20
                                11.592
MOTA
       2207 OW
               HOH
                     531 25.631
                                 32.409
MOTA
       2208 OW
               HOH
                     532 18.287
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                                         52.185 1.000 18.49
39.395 1.000 18.09
MOTA
       2209 OW
               HOH
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                                29.035
       2210 OW HOH
MOTA
                     534 10.797
                                 31.968
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MOTA
       2211 OW HOH
                     535 10.167
                                 24.890
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MOTA
       2212 OW HOH
                     536 23.530
                                 24.122
                                         58.531 1.000 20.39
ATOM
       2213 OW
               НОН
                     537 23.358
                                 12.639
                                         35.292 1.000 22.61
MOTA
       2214 OW
               нон
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MOTA
       2215 OW
                нон
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MOTA
       2216 OW
               HOH
                     540 18.515
                                 27.775
                                        40.042 1.000 22.23
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2217 OW HOH 541 21.233 20.367 33.996 1.000 21.45 2218 OW HOH 542 22.826 32.643 53.094 1.000 19.38 2219 OW HOH 543 19.670 22.387 35.310 1.000 20.05 ATOM ATOM ATOM ATOM 2220 OW 544 -13.591 21.996 61.494 1.000 49.93 545 21.295 11.783 55.080 1.000 20.04 HOH ATOM 2221 OW HOHHOH 545 21.295 11.783 55.080 1.000 20.04 HOH 546 5.431 2.533 51.677 1.000 28.11 HOH 547 17.311 25.489 32.148 1.000 24.38 HOH 548 17.427 7.744 33.008 1.000 20.78 HOH 549 11.656 23.874 58.194 1.000 23.39 HOH 550 8.037 14.987 53.326 1.000 33.52 HOH 551 1.354 14.574 33.889 1.000 21.05 HOH 552 11.203 20.116 63.686 1.000 24.59 HOH 553 2.671 21.240 34.245 1.000 34.51 ATOM 2222 OW ATOM 2223 OW ATOM 2224 OW ATOM 2225 OW 2226 OW HOH 550 8.037 ATOM 2227 OW HOH 551 1.354 ATOM ATOM 2228 OW HOH 2229 OW HOH ATOM 2230 OW HOH 554 6.339 ATOM 19.832 30.751 1.000 26.36 2231 OW HOH 555 26.611 24.519 ATOM 55.570 1.000 21.22 2232 OW HOH 556 27.669 17.156 ATOM 53.039 1.000 25.86 2233 OW HOH ATOM 557 -14.392 19.977 44.154 1.000 25.03 2234 OW HOH 558 14.828 32.652 51.443 1.000 25.23 MOTA 2235 OW HOH 559 17.937 7.207 ATOM 54.915 1.000 20.59 ATOM 2236 OW HOH 560 10.729 -8.875 31.499 1.000 24.65 2237 OW HOH 561 6.455 ATOM 2.298 42.613 1.000 22.74 2238 OW HOH 562 13.784 31.245 44.166 1.000 27.75 ATOM 2239 OW HOH 563 17.292 33.470 53.556 1.000 25.28 ATOM2240 OW HOH 564 11.210 1.109 49.697 1.000 23.33 2241 OW HOH 565 -11.339 25.246 41.370 1.000 26.08 2242 OW HOH 566 20.363 -8.375 38.242 1.000 30.07 2243 OW HOH 567 3.890 24.604 35.837 1.000 25.86 ATOM ATOM ATOM ATOM 2244 OW HOH 568 5.334 11.875 43.937 1.000 25.45 2245 OW HOH 569 7.861 22.385 64.046 1.000 28.98 2246 OW HOH 570 7.754 -1.508 30.848 1.000 24.72 2247 OW HOH 571 6.297 3.583 28.471 1.000 33.06 ATOM ATOM ATOM 2247 OW HOH 571 6.297 3.583 28.471 1.000 33.06 2248 OW HOH 572 -15.790 28.800 51.855 1.000 30.09 2249 OW HOH 573 -5.388 20.310 38.883 1.000 23.64 2250 OW HOH 574 17.657 21.059 29.053 1.000 24.31 2251 OW HOH 575 8.763 20.920 66.102 1.000 24.81 2252 OW HOH 576 10.135 27.617 58.357 1.000 25.12 2253 OW HOH 577 7.795 1.060 29.730 1.000 29.00 ATOM ATOM ATOM ATOM ATOM ATOM ATOM 2254 OW HOH 578 22.601 19.580 61.946 1.000 28.66 ATOM 2255 OW HOH 579 8.859 4.744 MOTA 27.898 1.000 26.12 48.882 1.000 26.29 35.057 1.000 23.31 ATOM 2256 OW HOH 580 4.937 3.932 2257 OW HOH 581 17.096 5.891 ATOM 2258 OW HOH 582 -16.337 31.047 64.719 1.000 54.01 MOTA 2259 OW HOH 583 7.652 24.826 52.106 1.000 27.23 2260 OW HOH 584 7.174 24.915 29.292 1.000 26.60 2261 OW HOH 585 23.452 10.614 55.439 1.000 26.42 2262 OW HOH 586 12.640 26.413 58.676 1.000 27.15 MOTA MOTA ATOM MOTA 2263 OW HOH 587 6.204 21.166 62.094 1.000 24.65 ATOM 2264 OW HOH 588 2.385 0.810 37.616 1.000 19.92 2265 OW HOH 589 32.930 28.236 45.738 1.000 38.29 2266 OW HOH 590 -12.045 28.716 45.065 1.000 30.46 ATOM ATOM ATOM 2266 OW HOH 590 -12.045 28.716 45.065 1.000 30.46 2267 OW HOH 591 0.219 13.612 36.120 1.000 27.12 2268 OW HOH 592 -2.525 3.881 43.344 1.000 26.67 2269 OW HOH 593 7.533 13.297 48.055 1.000 19.59 2270 OW HOH 594 -1.575 28.355 42.057 1.000 25.53 2271 OW HOH 595 11.209 -1.188 46.425 1.000 22.12 2272 OW HOH 596 5.684 -7.000 28.451 1.000 27.97 2273 OW HOH 597 28.868 19.406 51.825 1.000 27.72 2274 OW HOH 598 13.432 2.493 57.904 1.000 31.12 2275 OW HOH 599 8.196 7.483 27.148 1.000 29.99 MOTA ATOM MOTA ATOM MOTA ATOM ATOM MOTA 2275 OW HOH 599 8.196 ATOM 7.483 27.148 1.000 29.99 600 20.809 19.088 63.369 1.000 36.86 601 21.352 10.656 34.614 1.000 30.60 2276 OW HOH ATOM 2277 OW HOH ATOM

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2278 OW HOH MOTA 602 2.891 7.196 30.899 1.000 25.41 2279 OW ATOM HOH 26.496 34.561 1.000 35.71 603 8.260 ATOM 2280 OW HOH 604 22.300 13.959 31.378 1.000 32.53 ATOM 2281 OW HOH 605 15.689 35.750 48.870 1.000 31.17 ATOM 2282 OW HOH 606 7.219 15.638 30.914 1.000 27.80 ATOM 2283 OW нон 607 -3.237 14.604 47.092 1.000 20.96 ATOM 2284 OW нон 608 17.543 10.581 33.561 1.000 23.51 MOTA 2285 OW HOH 609 -1.899 36.370 44.261 1.000 32.64 2286 OW MOTA HOH 610 26.095 14.431 43.803 1.000 19.19 ATOM 2287 OW 611 27.664 41.954 1.000 26.48 49.981 1.000 24.70 HOH 13.183 ATOM 2288 OW HOH 612 4.302 34.604 2289 OW ATOM HOH 46.728 1.000 42.45 50.347 1.000 23.78 613 -15.580 27.012 ATOM 2290 OW HOH 614 1.615 35.544 2291 OW HOH ATOM 615 -10.137 34.259 49.033 1.000 23.94 57.657 1.000 39.32 2292 OW HOH MOTA 616 26.084 6.502 ATOM 2293 OW HOH 617 -15.962 20.656 46.340 1.000 25.94 2294 OW HOH ATOM 618 6.113 29.517 40.143 1.000 29.43 2295 OW HOH MOTA 619 19.797 4.627 51.313 1.000 27.15 2296 OW HOH ATOM 620 -1.748 11.315 48.716 1.000 21.83 ATOM 2297 OW HOH 621 11.099 44.259 1.000 27.15 34.289 ATOM 2298 OW HOH 622 28.352 37.877 1.000 41.48 14.351 2299 OW HOH ATOM 623 -2.826 36.968 57.149 1.000 32.75 2300 OW ATOM HOH 624 16.983 9.258 29.962 1.000 32.82 ATOM 2301 OW 625 16.780 29.213 HOH 38.384 1.000 27.96 2302 OW 626 1.632 17.213 627 33.536 23.640 ATOMHOH 33.689 1.000 23.17 2303 OW ATOM HOH 45.028 1.000 41.91 MOTA 2304 OW 628 23.821 6.059 HOH50.174 1.000 34.22 629 3.482 2.785 630 20.218 24.803 MOTA 2305 OW HOH 46.751 1.000 39.07 ATOM 2306 OW HOH 60.918 1.000 50.12 631 3.366 ATOM 2307 OW HOH 16.272 30.698 1.000 31.50 632 18.871 11.791 633 4.455 25.782 2308 OW HOH ATOM 31.384 1.000 30.78 ATOM 2309 OW HOH 58.823 1.000 32.14 2310 OW HOH ATOM 634 24.721 5.202 40.319 1.000 40.13 2311 OW HOH MOTA635 19.623 35.238 43.466 1.000 50.48 60.797 1.000 26.58 MOTA 2312 OW HOH 26.242 636 22.789 ATOM 2313 OW HOH 54.039 1.000 33.89 42.559 1.000 29.61 52.841 1.000 25.21 637 7.008 -4.809ATOM 2314 OW HOH 638 -15.821 18.362 2315 OW HOH ATOM 639 -11.847 15.711 ATOM 2316 OW HOH 640 -1.948 13.411 35.401 1.000 30.41 MOTA 2317 OW HOH 641 -14.293 21.937 42.145 1.000 27.58 MOTA 2318 OW HOH 642 18.216 20.839 66.863 1.000 31.23 MOTA 2319 OW HOH 643 9.836 36.288 48.178 1.000 44.21 2320 OW HOH 644 3.510 MOTA 16.168 66.253 1.000 33.82 MOTA 2321 OW HOH 645 7.571 33.398 41.687 1.000 37.96 2322 OW HOH 646 0.780 MOTA 21.844 36.729 1.000 31.71 ATOM 2323 OW HOH 647 21.244 -2.321 35.579 1.000 32.40 ATOM 2324 OW HOH 648 3.027 25.244 69.907 1.000 36.84 ATOM 2325 OW 649 1.129 HOH 25.273 66.516 1.000 35.42 ATOM 2326 OW HOH 650 14.646 7.560 60.327 1.000 46.42 2327 OW ATOM HOH 651 -8.287 26.381 37.998 1.000 29.17 ATOM 2328 OW HOH 652 10.153 23.548 67.703 1.000 31.50 MOTA 2329 OW HOH 653 28.906 22.258 38.969 1.000 32.66 ATOM 2330 OW 654 13.568 -4.482 31.517 1.000 26.94 HOH ATOM 2331 OW 655 -12.635 17.106 55.637 1.000 26.85 656 2.698 5.770 50.702 1.000 29.05 HOHMOTA 2332 OW HOH. 656 2.698 MOTA 2333 OW HOH657 -1.384 7.487 46.512 1.000 36.52 ATOM 2334 OW HOH 658 3.880 19.246 31.498 1.000 31.50 MOTA 2335 OW HOH 659 -1.400 31.406 23.260 64.001 1.000 56.62 MOTA 2336 OW 660 11.416 HOH 65.229 1.000 32.69 ATOM 2337 OW HOH 661 15.994 14.673 25.680 1.000 36.46 ATOM 2338 OW 662 28.572 21.242 HOH 53.423 1.000 39.06 H

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2339 OW HOH 663 19.354 0.465 ATOM 27.273 1.000 44.56 ATOM 2340 OW HOH 664 24.969 27.026 38.838 1.000 35.41 ATOM 2341 OW 665 24.294 7.488 HOH 55.914 1.000 32.97 ATOM 2342 OW HOH 666 19.540 7.882 31.178 1.000 30.04 ATOM 2343 OW HOH 667 -9.236 32.988 57.241 1.000 39.20 MOTA 2344 OW HOH 668 2.098 18.351 67.496 1.000 38.88 ATOM 2345 OW HOH 669 11.390 3.245 56.270 1.000 37.56 2346 OW ATOM HOH 670 -21.413 24.449 52.026 1.000 44.66 ATOM 2347 OW 671 -14.575 19.220 55.240 1.000 30.91 HOH672 32.112 25.958 43.051 1.000 33.34 ATOM 2348 OW HOH ATOM 2349 OW 673 -15.050 31.151 HOH 53.232 1.000 34.71 2350 OW HOH ATOM 674 2.941 30.245 1.000 34.63 34.757 1.000 49.17 -1.607ATOM 2351 OW 675 26.951 HOH 14.544 2352 OW ATOM нон 676 14.707 30.669 39.386 1.000 30.55 ATOM 2353 OW HOH 677 5.203 18.009 68.080 1.000 43.41 26.591 1.000 38.80 ATOM 2354 OW HOH 678 14.151 7.965 24.261 41.443 1.000 31.28 2.410 28.478 1.000 34.31 20.593 34.326 1.000 39.66 35.357 44.421 1.000 34.06 ATOM 2355 OW 679 24.470 HOH ATOM 2356 OW HOH 680 17.540 2357 OW HOH ATOM 681 25.992 20.593 ATOM 2358 OW HOH 682 13.802 35.357 ATOM 2359 OW HOH 683 1.087 2.355 45.456 1.000 35.39 2360 OW HOH 684 22.443 34.538 42.053 1.000 33.55 ATOM2361 OW HOH 685 4.419 ATOM 4.720 27.356 1.000 48.02 2362 OW HOH 686 -15.830 34.507 ATOM 51.877 1.000 50.63 2363 OW HOH 687 -15.217 29.490 48.887 1.000 33.54 ATOM MOTA HOH 688 36.808 21.183 2364 OW 46.206 1.000 44.97 MOTA 2365 OW HOH 689 3.756 1.312 29.272 1.000 35.16 ATOM 2366 OW HOH 690 18.802 13.646 27.901 1.000 30.08 2367 OW ATOM 691 6.997 HOH 17.521 29.313 1.000 47.70 ATOM 2368 OW 692 13.725 693 22.369 HOH16.327 69.105 1.000 36.97 ATOM 2369 OW HOH 22.161 60.503 1.000 44.09 ATOM 2370 OW 694 -5.429 31.620 695 19.351 23.082 HOH 42.219 1.000 33.40 2371 OW HOH ATOM 30.744 1.000 34.21 2372 OW HOH ATOM 696 6.897 22.414 29.376 1.000 36.59 MOTA 2373 OW HOH 697 28.700 7.809 0.679 57.304 1.000 38.35 2374 OW HOH ATOM 698 3.224 39.819 1.000 24.13 MOTA 2375 OW HOH 699 -4.634 33.717 62.593 1.000 32.26 ATOM 2376 OW HOH 700 32.423 17.018 43.200 1.000 43.20 25.228 68.342 1.000 39.95 16.477 28.976 1.000 31.75 34.067 46.117 1.000 49.40 31.390 65.371 1.000 39.12 MOTA 2377 OW HOH 701 12.119 ATOM 2378 OW HOH 702 9.307 2379 OW HOH 703 -11.313 34.067 ATOM MOTA 2380 OW HOH 704 7.774 2381 OW HOH 705 24.764 7.530 MOTA 2381 OW HOH 705 24.764 7.530 36.802 1.000 38.55 2382 OW HOH 706 -22.095 25.669 59.047 1.000 36.71 MOTA 2383 OW HOH 707 14.509 9.840 MOTA 68.854 1.000 50.38 2384 OW HOH 708 -10.129 28.722 42.036 1.000 38.92 MOTA MOTA 2385 OW HOH 709 29.011 34.910 48.390 1.000 35.29 ATOM 2386 OW HOH 710 15.822 31.612 42.021 1.000 33.61 ATOM 2387 OW HOH 711 -1.996 17.676 33.645 1.000 49.57 MOTA 2388 OW HOH 712 10.216 17.748 26.015 1.000 41.04 ATOM HOH 713 23.535 29.642 2389 OW 37.371 1.000 43.47 ATOM 2390 OW 714 20.488 -7.214 HOH 35.599 1.000 45.99 ATOM 2391 OW HOH 715 11.411 10.149 25.081 1.000 41.63 MOTA 2392 OW HOH 716 19.329 -4.258 34.139 1.000 42.50 ATOM 2393 OW HOH 717 13.688 26.799 66.321 1.000 43.74 ATOM 2394 OW 718 -10.751 33.064 HOH 54.747 1.000 40.47 MOTA 2395 OW 719 13.800 18.258 70.756 1.000 34.54 HOH MOTA 2396 OW HOH 720 17.151 5.815 28.003 1.000 40.80 MOTA 2397 OW HOH721 0.000 0.000 36.691 0.330 27.42 ATOM 2398 OW HOH722 0.000 0.000 41.559 0.330 37.77 2399 OW MOTA 723 15.314 7.549 HOH28.791 1.000 36.24

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MOTA	2400	OW	HOH	724	-1.663	19.944	39.196	1.000	33.87
ATOM	2401	OW	нон	725	19.289	24.195	33.321	1.000	32.28
ATOM	2402	OW	нон	726	0.000	0.000	31.798	0.330	50.38
ATOM	2403	OW	НОН	727	-1.223	38.165	59.229	1.000	31.24
ATOM	2404	OW	НОН	728	22.035	38.254	45.742	1.000	48.21
ATOM	2405	OW	НОН	729	28.388	16.248	63.044	1.000	31.59
ATOM	2406	OW	нон	730	0.000	0.000	45.995	0.330	36.14
ATOM	2407	OW	нон			29.007			
ATOM	2408	OW	нон	732	5.297		40.091	1.000	36.08
ATOM	2400	OW	НОН	732		15.835	27.318	1.000	41.53
ATOM	2410	OW			17.347	10.778	27.373	1.000	35.27
			HOH	734	29.417	14.607	53.127	1.000	
ATOM	2411	OM	HOH		4.222	-8.636	27.012	1.000	35.22
ATOM	2412	OW	HOH			17.712	62.813	1.000	34.43
ATOM	2413	OW	HOH	737	13.960	-10.203	55.259	1.000	31.79
ATOM	2414	OW	HOH	738	11.831	-1.522	49.308	1.000	25.22
ATOM	2415	OW	НОН			4.247	29.596	1.000	38.64
MOTA	2416	OW	НОН	740	10.959	13.759	25.528	1.000	61.86
ATOM	2417	OM	HOH	741	0.864	17.227	30.557	1.000	50.71
ATOM	2418	OW	HOH	742	31.755	18.949	52.065	1.000	40.48
MOTA	2419	OM	HOH	743	21.678	-0.485	28.218	1.000	43.23
ATOM	2420	OW	HOH	744	10.583	16.397	75.211	1.000	45.04
ATOM	2421	OW	HOH	745	7.480	7.996	78.287	1.000	57.64
MOTA	2422	OM	HOH	746	24.067	35.122	40.297	1.000	41.95
ATOM	2423	OW	HOH	747	7.804	10.269	78.332	1.000	49.63
ATOM	2424	WO	HOH	748	22.131	40.645	45.806	1,000	49.69
ATOM	2425	OW	HOH	749	14.850	-4.647	33.872	1.000	42.88
ATOM	2426	OW	нон	750	-12.930	32.504	55.211	1.000	37.15
ATOM	2427	OW	нон	751	-4.832	35.986	43.333	1.000	44.39
ATOM	2428	OW	нон	752	19.834	33.566	56.449	1.000	31.56
ATOM	2429	OW	нон	753	3.363	22.310	29.844	1.000	
ATOM	2430	OW	нон			4.030	34.174	1.000	51.90
ATOM	2431	OW	нон	755	28.036	35.859	46.448	1.000	39.50
ATOM	2432	OW	НОН	756	-12.951	16.294	61.787	1.000	40.94
ATOM	2433	OW	нон	757	-10.870	26.452	38.737	1.000	44.85
ATOM	2434	OW	нон	758	13.216	12.896	70.729	1.000	63.42
ATOM	2435		нон		-0.403			1.000	38.96
ATOM			НОН		-7.025	21.161	74.990		
ATOM	2437	OW	НОН			32.526	64.316	1.000	39.64
				761	-15.459	19.739	58.090	1.000	40.84
ATOM	2438	OM	HOH	762	-4.964	36.577	59.068	1.000	48.64
ATOM	2439	WO	НОН	763	26.807	35.717	50.036	1.000	43.54
ATOM	2440	OW	нон	764	19.542	7.083	65.538	1.000	41.41
ATOM	2441	OW	нон	765	3.709	35.837		1.000	33.78
ATOM	2442	OW	НОН	766	0.431	33.688	40.172	1.000	36.91
ATOM	2443	OW	HOH	767	18.620	5.064	64.617	1.000	
ATOM	2444	OW	HOH	768	35.526	19.792	41.322	1.000	52.54
ATOM	2445	OW	HOH			7.789	67.717	1.000	
ATOM	2446	OW	HOH			12.048	26.149	1.000	40.08
MOTA	2447	OW	HOH	771	20.245	35.637	53.927	1.000	52.16
MOTA	2448	OW	HOH	772	-20.588	25.640	61.573	1.000	58.60
ATOM	2449	OW	HOH	7 73	1.556	37.342	52.171	1.000	36.23
ATOM	2450	OW	нон	774	8.340	0.668	49.382	1.0001	107.24
MOTA	2451	OW	HOH	775	27.160	2.372	34.466	1.000	59.84
ATOM	2452	OW	HOH	776	6.575	19.271	25.545	1.000	36.68

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ATOM	2453	OW	HOH	777	-17.605	29.205	62.661	1.000	56.83
ATOM	2454	OW	HOH	778	7.616	6.902	24.722		61.34
MOTA	2455	OW	HOH	779	19.749	10.700	68.006	1.000	65.22
MOTA	2456	W	НОН	780	7.281	-5.270	50.090	1.000	50.00
ATOM	2457	W	HOH	781		28.483	40.515	1.000	50.00
ATOM	2458	W	нон	782	9.990	17.263	38.636		50.00
ATOM	2459	W	HOH	783	5.767	-2.331	28.939	1.000	50.00
ATOM	2460	W	НОН	784		-0.118	24.984	1.000	50.00
ATOM	2461	W	НОН	785	24.442	7.952	47.994	1.000	50.00
ATOM	2462	W	НОН	786	14.251	36.889	46.491		50.00
ATOM	2463	W	НОН	787		26.477	33.851		50.00
ATOM	2464	W	НОН		-11.816		40.795	1.000	50.00
ATOM	2465	W	НОН		-2.531	5.579	45.829	1.000	50.00
ATOM	2466	W	НОН		-13.002	32.034	46.612	1.000	
ATOM	2467	W	НОН		2.230	3.555	48.985		50.00
ATOM	2468	W	НОН		9.397	13.464	28.121	1.000	50.00
ATOM	2469	W	НОН	793	28.257	10.442			50.00
ATOM	2470	W	НОН		4.652		42.781	1.000	50.00
ATOM	2471	W	НОН		5.977	17.944	59.241	1.000	50.00
ATOM	2472	W	НОН	796		15.287	79.554	1.000	50.00
ATOM	2473	W			30.501	11.852	47.616	1.000	50.00
ATOM	2473		HOH	797	5.625	14.258	54.367	1.000	50.00
ATOM		W	HOH	798	23.942	20.228	33.277	1.000	50.00
	2475 2476	W	нон	799	10.164	14.642	58.997	1.000	50.00
ATOM ATOM		W	HOH	800	7.807	31.943	52.999	1.000	50.00
	2477	W	HOH	801	23.377	9.361	34.817		50.00
ATOM	2478	W	HOH		21.193	9.722	32.004	1.000	50.00
ATOM	2479	W	НОН	803	34.928	14.644	46.038	1.000	50.00
ATOM	2480	W	НОН		29.073	16.684	34.445	1.000	50.00
ATOM	2481	W	НОН	805	7.008	-2.049	51.872	1.000	50.00
ATOM	2482	W	НОН	806	25.363	7.860	45.531	1.000	50.00
ATOM	2483	W	HOH		30.704	8.207	55.971	1.000	50.00
ATOM	2484	W	HOH	808	33.072	24.900	40.599	1.000	50.00
ATOM	2485	W	HOH	809	-15.577	19.225	63.152	1.000	50.00
ATOM	2486	W	HOH	810	6.072	18.137	23.603	1.000	50.00
ATOM	2487	W	НОН	811	-7.214	39.940	55.639	1.000	50.00
ATOM	2488	W	HOH		5.509	18.517	74.919	1.000	50.00
ATOM	2489	W	HOH	813	33.845	9.908	56.672	1.000	50.00
MOTA	2490	W	HOH	814	0.421	35.779	42.931	1.000	50.00
MOTA	2491	W	HOH	815	35.282	21.705	48.656	1.000	50.00
MOTA	2492	W	НОН	816	39.344	22.173	46.871	1.000	50.00
ATOM	2493	W	HOH	817	-5.192	39.820	60.056	1.000	50.00
MOTA	2494	W	HOH	818	30.199	13.039	33.383	1.000	
MOTA	2495	W	HOH	819	-4.860	36.454	61.731		
ATOM	2496	W	HOH	820	-14.599	17.407	58.382		
ATOM	2497	W	HOH	821	1.340	-0.111	41.711		
ATOM	2498	W	нон		34.512	23.218	52.108		50.00
MOTA	2499	W	нон		32.136	12.571	52.190		50.00
ATOM	2500	W	нон		13.525	-6.549			50.00
ATOM	2501	W	нон		6.072	-4.141		1.000	
					· - · -				20.00

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STRUCTURE B

ATOM 1 ANISOU 2 ANISOU 3 ATOM 3 ANISOU 3 ATOM 4 ANISOU 4 ATOM 5 ANISOU 6 ANISOU 6 ATOM 7 ANISOU 7 ATOM 8 ANISOU 7 ATOM 8 ANISOU 7 ATOM 10 ANISOU 11 ATOM 12 ANISOU 12 ATOM 13 ATOM 14 ANISOU 14 ANISOU 14 ANISOU 14 ANISOU 15 ATOM 16 ANISOU 15 ATOM 16 ANISOU 16 ATOM 17 ANISOU 17 ANISOU 16 ATOM 17 ANISOU 17 ANISOU 16 ATOM 17 ANISOU 20 ANISOU 20 ANISOU 21 ANISOU 21 ANISOU 22 ANISOU 22 ANISOU 23 ANISOU 24 ANISOU 25 ANISOU 26 ANISOU 26 ANISOU 27 ANISOU 27 ANISOU 27	CA CB CB CG OD1 OD2 OD2 CC OON NCA CB CG OG1 CG2 CC OON NCA CB CG2 CC OON NCA CB CG2 CC OON NCA CB CG1 CG2 CC OON NCA CB CG1 CG2 CC OON NCA CB CG1 CG2 CC CO OON NCA CB CG1 CG2 CC OON NCA CB CG1 CG1	THR	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	31.030 5663 30.206 6595 28.694 7003 27.852 8632 31.587 6204 31.239 7381 33.170 4533 32.156 6441 31.485 3460 30.759 4439 31.206 380.519 4511 29.325 5866 30.363 5994 29.275 4131 27.046 4602 28.467 4731 27.046 4602 26.447 7170 26.629 27.153 9604 26.240 4535 27.153 9604 26.240 4535 27.153 9604 26.240 4535 27.153 9604 26.240 4535 27.163 28.805 29.275 26.240 27.153 26.240 26.250 2	11.882 12.892 12.690 3775 11.848 3962 11.584 3912 13.367 4752 12.847 5242 16.034 17.2847 14.646 15.478 16.918 17.689 17.689 17.689 17.689 17.689 17.689 17.689 17.689 18.181 18.3634 17.64 17.64 17.64 17.64 17.64 17.64 17.64 17.64 17.64 17.64 18.64 18.64 18.64 19.12 18.64 19.12 18.63 19.12 19.1	9809 86 9246 59 4424 20 4677 99 8854 65 58.38 89 60.38 81 9567 22 51138 81 958.70 96 598.21 09 598.21 09 598.21 09 598.21 09 599.22 21 599.22 21 599.33 3 599.34 3 599.3	1.000 5 0.9 6 1113 -2217 - 5 5 4 1.000 5 1.63 691 -1891 1 6 9 1.000 40.50 833 -1535 - 4 6 0 1.000 45.32 -239 -653 - 1702 1.000 5 2.14 287 -2128 - 6 3 1.000 5 2.9 2 1417 -4224 5 1 9 1.000 5 7.78 34 -1912 - 8 1 1 1.000 5 4.62 137 -2012 - 6 1 7 1.000 43.5 2 474 -2350 4 7 1.000 41.69 -309 -2603 - 3 1 1.000 3 7.8 9 -304 -3473 2 6 6 1.000 3 9.5 9 15 -3218 5 8 9 1.000 45.10 -553 -1950 - 6 2 5 1.000 42.05 -465 -3788 1 4 5 1.000 33.8 4 -59 -1682 - 1 2 2 1.000 29.2 5 658 -390 - 6 1 5 1.000 29.4 1 907 -2076 - 2 8 4 1.000 29.4 1 907 -2076 - 2 8 4 1.000 29.4 1 907 -2076 - 2 8 4 1.000 29.4 1 907 -2076 - 2 8 4 1.000 3 6.5 1 -791 -1996 5 2 1.000 42.4 5 -920 -1251 3 8 3 1.000 50.2 6 -602 -733 - 3 3 3 1.000 29.0 1 738 -1079 9 9 1.000 35.8 2 390 524 -1246 1.000 24.9 8 542 -2040 - 9 8 6 1.000 23.9 7 344 -1563 - 3 7 5 1.000 26.7 7 651 -988 - 9 2 3 1.000 32.6 2 195 -2081 - 1 1 3	
ANISOU 25 ATOM 26 ANISOU 26 ATOM 27 ANISOU 27 ATOM 28 ANISOU 28 ATOM 29 ANISOU 29 ATOM 30 ANISOU 30	CA CB CB OG1 OG2 CG2 C C	THR	4 4 4 4 4 4 4 4 4 4	3437 27.183 2636 28.050 3398 26.429 2373 25.325 3090 25.738 2668	2426 19.650 2429 19.484 2812 20.942 2692 18.577 2760 18.264 2629	3244 60.408 5105 61.551 6184 60.663 4967 59.097 2374 57.980 2902	344 -1563 - 375 1.000 26.77 651 -988 - 923 1.000 32.62 195 -2081 -113 1.000 26.40 533 -573 -1570 1.000 21.64 368 -750 - 20 1.000 21.58 246 -560 - 659	
ATOM 30	0	THR	4	25.738	18.264	57.980	1.000 21.58	

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ANISOU 31 VAL 5 2505 2021 -613 -630 - 162 N 1508 CA VAL 5 23.211 19.385 58.211 1.000 14.80 ATOM -594 -473 - 87 ANISOU 32 CAVAL 5 2463 1893 1266 58.606 1.000 16.09 СВ VAL 5 21.742 MOTA 33 19.402 ANISOU 33 CB VAL 5 2476 1881 1757 -412 -406 5 0 2 CG1 VAL 5 20.855 57.447 1.000 14.91 19.846 ATOM 5 ANISOU 34 CG1 VAL 2468 1859 1337 9 -102 197 CG2 VAL 5 21.310 MOTA 35 17.994 59.074 1.000 21.15 CG2 VAL ANISOU 35 5 3015 2345 2677 -700 -418 1198 С VAL 5 20.762 57.694 1.000 17.70 ATOM 36 23.639 ANISOU 36 С 5 VAL 2893 2085 1749 -1137 -713 1 0 3 23.532 37 5 21.759 58.419 1.000 17.35 MOTA 0 VAL 5 ANISOU 37 0 VAL 2566 1978 2050 -698 -650 1 0 5 38 И PRO 6 24.150 20.845 56.479 1.000 13.23 MOTA ANISOU 38 1597 N PRO б 1334 2097 -162 -668 4 0 9 39 PRO 6 19.770 55.484 1.000 15.56 ATOM CD 24.302 6 -309 -383 2 7 7 ANISOU 39 CD PRO 1887 1850 2176 40 CAPRO 6 22.137 56.005 1.000 14.49 MOTA 24.667 ANISOU 40 6 CAPRO 1332 1740 2432 -218 -536 5 2 2 6 21.722 54.847 1.000 18.21 ATOM 41 CB PRO 25.571 ANISOU 41 CB PRÓ 6 2294 1740 2886 -224 130 434 20.378 54.409 1.000 20.37 MOTA 42 CG PRO 6 25.132 2632 PRO 2399 -107838-61ANISOU 42 CG 6 2708 23.091 55.510 1.000 14.59 MOTA 43 C PRO 6 23.576 ANISOU 43 C PRO 1712 -406 -786698 6 1388 2443 MOTA 440 PRO 22.408 22.743 55.295 1.000 13.06 6 ANISOU 44 0 PRO 6 1298 1547 -283 -596 1 5 2118 THR 7 24.048 24.326 55.313 1.000 14.56 ATOM 45 Ν ANISOU 45 Ν THR 7 1393 1678 2463 -380 -565 5 8 7 7 23.288 25.428 54.771 1.000 13.28 ATOM 46 CATHR1584 -469 -734 4 4 0 ANISOU 46 CATHR 7 1463 1998 47 CB THR 7 23.121 26.572 55.799 1.000 14.44 ATOM 7 ANISOU 47 CB THR 1652 1905 -348 -1257 3 2 9 1927 7 7 ATOM 48 OG1 THR 22.454 26.102 56.998 1.000 18.44 OG1 THR -333 -829 1 7 6 ANISOU 48 3136 2013 1858 22.290 27.719 55.261 1.000 14.98 MOTA 49 CG2 THR 7 7 ANISOU 49 CG2 THR 1390 1788 2513 -213 -727 4 1 2 7 26.005 53.539 1.000 14.62 23.973 ATOM 50 C THR 7 ANISOU 50 C 2212 -355 -693 7 0 4 THR 1144 2200 26.257 53.600 1.000 17.21 7 25.192 MOTA 51 0 THR 7 -641 -840 9 7 5 ANISOU 51 2515 2738 0 THR 1284 MOTA 26.222 52.472 1.000 12.32 52 8 23.211 Ν PHE ANISOU 52 1165 1596 1919 -314 -534 3 7 0 PHE 8 Ν MOTA 53 CAPHE 8 23.692 26.869 51.283 1.000 13.31 ANISOU 53 -295 3 4 3 CAPHE 8 1554 1531 1971 -60 23.724 25.933 50.067 1.000 13.71 ATOM CB 8 54 PHE ANISOU 54 CB PHE 8 1479 1705 2025 -136 -232 2 3 4 24.635 24.746 50.258 1.000 13.68 ATOM 55 CG PHE 8 ANISOU 55 1225 -185 8 155 CG PHE 8 1716 2257 CD1 PHE 24.147 23.503 50.628 1.000 14.10 ATOM 56 8 ANISOU 56 CD1 PHE 8 1317 1710 2329 -93 231 221 26.006 24.882 50.079 1.000 17.52 MOTA 57 CD2 PHE 8 ANISOU 57 CD2 PHE 8 1239 2282 3134 -234 -56 MOTA 58 CE1 PHE 8 24.984 22.420 50.812 1.000 15.39 ANISOU 58 CE1 PHE 8 1473 1878 2497 -11 242 481 23.807 50.271 1.000 17.73 MOTA CE2 PHE 59 8 26,840 ANISOU 59 -157 -143 4 2 3 CE2 PHE 1179 2259 8 3301 MOTA 60 CZPHE 26.348 22.567 50.654 1.000 17.12 8 24 - 382 978 ANISOU 60 CZPHE 8 1310 2437 2757 ATOM 61 C 8 22.821 28.073 50.909 1.000 12.76 PHE ANISOU 61 C -164 -145 4 4 2 PHE 8 1401 1513 1935

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2319

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2650

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2158

1583

2104

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33.679 50.059 1.000 29.26

30.402 44.882 1.000 17.16

30.317 44.032 1.000 18.88

29.441 45.049 1.000 17.32

28.252 44.189 1.000 14.00

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-720 -1365 797

-1279 -1848 476

-624 -715 4 8 1

-1004 -306 8 9 9

-659 -386 9 4

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ATOM 62 0 PHE 8 21.602 28.033 51.079 1.000 13.18 ANISOU 62 PHE 8 1392 1295 2322 -256 -400 3 6 4 MOTA 63 SER 9 23.478 29.096 50.394 1.000 13.03 SER 9 ANISOU 63 1722 1636 1593 -565 -601 4 9 0 SER 9 MOTA 64 CA22.861 30.224 49.718 1.000 12.55 ANISOU 64 9 CA SER 1591 1468 1708 -392 -438 3 1 5 ATOM 65 СВ 9 SER 23.743 31.472 49.761 1.000 15.41 ANISOU 65 9 CBSER 2385 1833 1637 -915 -1057 783 MOTA 66 OG 9 SER 23.138 32.539 49.007 1.000 17.99 OG ANISOU 66 SER 9 2504 1721 2611 -718 -999 9 2 4 MOTA 67 С SER 9 22.520 29.868 48.276 1.000 12.72 SER 9 ANISOU 67 C 2040 1187 1606 -411 -576 4 7 6 SER 9 ATOM 68 0 23.397 29.495 47.478 1.000 16.18 9 ANISOU 68 0 SER 2265 2053 1830 **-465 -381** 7 3 10 MOTA 69 LEU Ν 21.229 29.982 47.968 1.000 14.19 ANISOU 69 N LEU 10 2154 1488 1750 -301 -699 1 7 4 MOTA 70 CALEU 10 20.798 29.714 46.596 1.000 14.62 ANISOU 70 CALEU 10 2243 1579 1734 -184 -784 2 2 4 71 ATOM СВ LEU 10 19.291 29.883 46.436 1.000 14.72 ANISOU 71 СВ LEU 1657 10 2222 1714 -142 -657 -168 ATOM 72 СG LEU 10 18.693 29.633 45.050 1.000 14.10 ANISOU 72 CG LEU 10 2087 1557 1713 -702 -695 1 4 5 ATOM 73 CD1 LEU 18.986 28.214 44.582 1.000 16.23 10 ANISOU 73 CD1 LEU 10 2994 1578 -554 -1132 8 7 1595 CD2 LEU ATOM 10 17.198 29.913 44.997 1.000 21.82 ANISOU 74 CD2 LEU 10 2180 2904 3206 -421 -1151 -518 ATOM 75 С LEU 10 21.531 30.639 45.626 1.000 15.87 ANISOU 75 С LEU 10 2449 1785 1796 -491 -844 3 1 4 ATOM 76 0 LEU 10 21.962 30.199 44.553 1.000 16.33 ANISOU 76 0 LEU 10 2607 1816 1780 -601 -829 2 7 6 ATOM 77 N ALA 31.917 45.986 1.000 17.17 11 21.669 ANISOU 77 N ALA 11 2521 1889 2115 -607 -548 1 3 9 CA ALA 11 ATOM 78 22.335 32.912 45.129 1.000 16.56 ANISOU 78 ALA 11 CA 2377 1884 2029 -732 -1033 3 0 2 ATOM 79 CBALA 11 22.199 34.259 45.805 1.000 20.05 11 ANISOU 79 CB ALA 3210 1877 2529 -670 -674 2 5 9 11 ATOM 80 С ALA 23.786 32.535 44.831 1.000 16.33 ANISOU 80 С ALA2319 2255 1629 -754 -988 4 3 4 11 MOTA 81 0 ALA 24.260 32.587 43.677 1.000 19.66 ANISOU 81 3115 0 ALA 11 2559 1795 -947 -560 6 1 9 ATOM 82 Ν GLU 12 24.558 32.085 45.810 1.000 17.28 ANISOU 82 GLU N 12 2686 1994 1884 -454 -1087 3 9 0 MOTA 83 CA GLU 12 25.931 31.654 45.752 1.000 16.34 ANISOU 83 CA GLU 12 2703 1674 1831 -474 -889 1 0 3 3 ATOM 84 CB GLU 12 26.527 31.477 47.158 1.000 16.09 ANISOU 84 CB GLU 12 2440 1867 1808 -770 -820 1 0 5 8 ATOM CG 8.5 GLU 32.802 47.915 1.000 18.90 12 26.633 ANISOU 85 CG GLU 12 2717 2127 2335 -1216 -1090 788 MOTA 86 CD GLU 12 27.115 32.657 49.342 1.000 21.17

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CA LEU 13
CB LEU 13
CB LEU 13
CG LEU 13
CG LEU 13
CD1 LEU 13
CD1 LEU 13
CD2 LEU 13
CD2 LEU 13
CD2 LEU 13 ANISOU 92 1734 1873 1713 -140 -170 4 9 8 MOTA 93 24.003 27.248 44.620 1,000 15.37 ANISOU 93 2205 1838 1795 -375 -149 4 6 5 24.154 26.554 45.967 1.000 14.52 MOTA 94 1913 ANISOU 94 1803 1799 -280 -204 4 4 2 ATOM 95 22.934 25.680 46.193 1.000 15.15 ANISOU 95 2174 1817 1766 -433 185 1 25.411 25.690 46.067 1.000 17.54 -433 185 175 ATOM 96 ANISOU 96 2119 2043 2502 -38 -419 2 7 0 24.876 28.626 42.725 1.000 16.54 LEU 13 ATOM 97 С ANISOU 97 С 13 LEU 2510 2062 1710 -222 -93 565 ATOM 98 0 25.548 28.122 41.821 1.000 18.28 LEU 13 ANISOU 98 O LEU 13 2685 2514 1748 -687 75 2 5 9 GLN 14 MOTA 99 N 23.945 29.534 42.472 1.000 16.86 ANISOU 99 GLN 14 N 1970 2337 -557 -683 8 3 8 2100 100 CA GLN 14 ATOM 23.657 30.015 41.132 1.000 18.63 ANISOU 100 CA GLN 14 2761 2404 1915 -610 -802 5 6 8 101 CB GLN 14 ATOM 22.421 30.923 41.130 1.000 19.39 ANISOU 101 CB GLN 14 3166 2176 2025 -392 -918 9 7 7 ATOM 102 CG GLN 14 21.108 30.250 41.460 1.000 19.00 ANISOU 102 CG GLN 14 2879 2383 1957 -209 -725 4 6 0 CD GLN 14 MOTA 103 19.974 31.227 41.766 1.000 18.83 CD GLN 14 ANISOU 103 3139 2118 1897 -6 -1229 4 9 4 OE1 GLN 14 20.177 32.317 42.314 1.000 26.10 ATOM 104 ANISOU 104 OE1 GLN 14 3928 2407 3582 -98 -1172 -241 14 ATOM 105 NE2 GLN 18.745 30.823 41.411 1.000 20.94 ANISOU 105 NE2 GLN 2900 2716 2340 -149 -840 4 24.804 30.812 40.525 1.000 20.40 14-149 -840 4 5 4 ATOM 106 С GLN 14 ANISOU 106 C GLN3226 2458 2065 -795 -712 9 24.812 30.951 39.311 1.000 30.48 14 -795 -712 9 3 7 107 0 ATOM GLN 14 ANISOU 107 O GLN 5089 4340 2152 -235. 25.734 31.309 41.329 1.000 20.35 2030 -1067 -240 4 14 5089 -2337 -898 1211 108 N ATOM GLN15 ANISOU 108 N GLN15 -1067 -240 4 9 7 26.909 32.041 40.884 1.000 21.88 109 CA GLN 15 ATOM CA GLN 15 ANISOU 109 3184 3230 1901 -1152 -299 7 8 8 110 CB GLN 15 27.288 33.100 41.920 1.000 22.20 ATOM ANISOU 110 CB GLN 15 2720 3162 2551 -1131 -770 6 9 1 111 CG GLN 15 26.450 34.358 41.954 1.000 25.73 ATOM ANISOU 111 CG GLN 15 4496 2735 2545 -821 -233 1 2 6 9 26.325 35.021 43.306 1.000 35.76 ATOM 112 CD GLN 15 ANISOU 112 CD GLN 15 6010 3945 3631 -643 -229 - 135 MOTA 113 OE1 GLN 15 27.145 34.884 44.225 1.000 49.13 ANISOU 113 OE1 GLN 15 8425 5866 4378 -2857 -2197 - 564 MOTA 114 NE2 GLN 15 25.255 35.812 43.489 1.000 51.85 ANISOU 114 NE2 GLN 15 7190 5567 6945 62 3066 107 115 C ATOM GLN 15 28.069 31.079 40.625 1.000 23.93 ANISOU 115 C GLN 15 3451 3513 2127 -990 145 884 ATOM 116 0 GLN 15 29.177 31.448 40.213 1.000 28.95 ANISOU 116 O GLN 15 3535 4619 2845 -899 510 1225 ATOM 117 N GLY 16 27.828 29.794 40.891 1.000 25.86 16 ANISOU 117 N GLY4089 3282 2457 -889 -36 4 28.812 28.763 40.649 1.000 29.00 -889 -36 469 16 MOTA 118 CA GLY ANISOU 118 GLY 16 CA 4785 3562 2671 -677 765 255 ATOM 16 119 GLY 29.741 28.546 41.814 1.000 25.45 ANISOU 119 С GLY 16 3427 3490 2754 -264 1422 673 ATOM 120 0 GLY 30.805 27.955 41.625 1.000 29.63 16 ANISOU 120 O GLY 16 3925 3267 4068 1997 5 2 3 -66 121 N ATOM LEU 17 29.387 28.979 43.015 1.000 22.50 ANISOU 121 N LEU 17 3266 2713 2569 923 733 -39 MOTA 122 CA LEU 17 30.234 28.727 44.172 1.000 21.73 ANISOU 122 CALEU 17 2931 2299 3025 -282 867 748

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CB LEU 17 CB LEU 17 29.921 45.132 1.000 21.23 123 30.124 LEU -620 669 711 ANISOU 123 2137 2858 3071 CG 17 31.274 44.431 1.000 26.12 124 LEU 30.354 ATOM CG LEU 17 ANISOU 124 2708 -889 1342 9 3 1 2965 4253 125 CD1 LEU 17 29.962 32.444 45.305 1.000 29.81 MOTA ANISOU 125 CD1 LEU 17 2515 2924 5885 -396 464 303 31.350 43.974 1.000 32.84 CD2 LEU 17 126 31.808 ATOM ANISOU 126 CD2 LEU 17 2845 3703 5930 -281 1871 2114 127 С LEU 17 29.886 27.456 44.936 1.000 19.36 ATOM С ANISOU 127 LEU 2455 17 2081 2819 -239 545 580 128 0 LEU 17 26.920 44.848 1.000 21.11 MOTA 28.773 ANISOU 128 0 LEU 17 3004 2284 2734 -444 107 1055 129 ATOM Ν HIS 18 30.838 26.952 45.706 1.000 21.02 18 N ANISOU 129 HIS 2752 2124 3109 -314 193 491 18 130 CA HIS 30.678 25.814 46.615 1.000 18.11 ATOM 18 18 ANISOU 130 HIS 2996 -460 -28 361 CA1569 2315 MOTA 131 CB HIS 29.655 26.149 47.702 1.000 21.25 ANISOU 131 CB HIS 18 1731 3332 3010 282 354 -45 HIS 132 CG 29.796 27.515 48.283 1.000 23.28 MOTA 18 18 ANISOU 132 CG HIS 2234 3612 2999 211 -46 -20 CD2 HIS 133 18 28.535 48.344 1.000 24.53 ATOM 28.898 ANISOU 133 41 4 4 0 CD2 HIS 18 3112 3479 2728 532 134 30.940 27.977 48.895 1.000 26.72 ATOM ND1 HIS 18 ANISOU 134 ND1 HIS 18 2938 4039 3173 -151 -569 3 8 ATOM 135 CE1 HIS 18 30.756 29.218 49.307 1.000 29.80 ANISOU 135 -542 -562 2 3 7 CE1 HIS 18 4476 3775 3071 136 29.524 29.581 48.985 1.000 30.03 ATOM NE2 HIS 18 ANISOU 136 NE2 HIS 18 4752 3282 3377 216 -148 3 3 8 30.266 24.528 45.917 1.000 18.57 ATOM 137 HIS 18 С 1943 3084 2028 -951 30 5 9 0 29.594 23.682 46.532 1.000 19.92 ANISOU 137 C HIS -951 30 5 9 0 18 ATOM 138 0 HIS 18 ANISOU 138 HIS 2493 -777 -87 995 0 18 1949 3125 30.647 24.340 44.658 1.000 19.24 ATOM 139 GLN19 N ANISOU 139 N GLN 19 2329 2700 2282 -256 298 494 30.119 23.206 43.908 1.000 21.51 MOTA 140 CA GLN 19 ANISOU 140 2431 -228 597 318 CAGLN19 3249 2492 30.446 23.307 42.406 1.000 22.89 ATOM CB 19 141 ${\tt GLN}$ ANISOU 141 CB GLN3058 2408 19 3231 -148 463 244 ATOM 142 CG GLN 19 29.738 24.453 41.698 1.000 25.83 3445 ANISOU 142 3712 2658 CG GLN19 -384 -407 5 6 8 MOTA 143 CD GLN19 28.223 24.470 41.747 1.000 31.56 ANISOU 143 GLN CD19 3439 4722 3832 -252 -988 3 5 7 ATOM 144OE1 GLN 19 27.521 23.640 41.153 1.000 38.51 ANISOU 144 7115 OE1 GLN 19 3869 3649 377 -3045 686 ATOM 145 NE2 GLN 19 27.621 25.433 42.475 1.000 33.32 ANISOU 145 NE2 GLN 3303 5695 19 3663 647 -1109 4 4 9 30.578 21.873 44.485 1.000 20.32 ATOM 146 C GLN 19 ANISOU 146 С GLN 19 2224 2710 2785 -60 514 394 19 MOTA 147 0 GLN 29.806 20.900 44.473 1.000 19.08 ANISOU 147 19 1888 2451 2910 221 257 743 0 GLN 31.800 21.761 44.999 1.000 24.09 MOTA 148 N ASP 20 ANISOU 148 -773 -507 4 1 5 N ASP 20 3001 3507 2645 ATOM 149 CAASP 32.268 20.498 45.553 1.000 21.82 20 -327 -58 357 ANISOU 149 CA ASP 20 1707 3811 2774 MOTA 150 33.780 20.527 45.779 1.000 26.34 CB ASP 20 ANISOU 150 ASP 20 1594 4552 -962 236 490 CB 3863 151 ATOM CG ASP 20 34.596 20.517 44.503 1.000 34.45 ANISOU 151 CG ASP 20 2531 5859 4701 -1208 1213 - 280 34.177 152 OD1 ASP 20 19.982 43.457 1.000 33.11 ANISOU 152 OD1 ASP 20 3768 4173 4640 -311 1233 -375ATOM 153 OD2 ASP 20 35.725 21.056 44.532 1.000 49.71

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ANISOU 153 OD2 ASP 20 3445 9922 5519 -3116 1710 5 3 154 C 20 31.538 20.179 46.862 1.000 21.03 ASP MOTA ANISOU 154 C 1876 ASP 20 2702 -231 616 388 3412 ATOM 155 0 ASP 20 31.118 19.038 47.075 1.000 20.80 ANISOU 155 O ASP 20 1162 2583 4157 -72 -139 5 5 0 156 N GLU 21 31.359 21.177 47.729 1.000 17.88 ATOM ANISOU 156 GLU 21 1218 2751 2824 -263 -148 5 1 1 157 CA GLU 30.599 20.999 MOTA 21 48.965 1.000 16.80 CA GLU ANISOU 157 21 1128 2173 3083 -96 46 3 9 4 158 СВ GLU 21 30.654 22.304 49.781 1.000 20.23 MOTA ANISOU 158 CB GLU 21 1366 2620 3701 5 -262 -210 ATOM 159 CG GLU 21 32.040 22.669 50.307 1.000 24.60 ANISOU 159 CG GLU 21 1660 3325 4359 -221 -654 - 301 160 CD GLU 21 32.860 ATOM 23.565 49.402 1.000 28.46 ANISOU 160 CD GLU 21 1191 4348 5275 -498 -1597 1125 MOTA 161 OE1 GLU 21 33.751 24.294 49.919 1.000 31.17 ANISOU 161 OE1 GLU 21 2360 4428 5057 -1039 -1094 3 4 9 OE2 GLU 32.664 23.590 48.171 1.000 31.16 162 21 ATOM ANISOU 162 OE2 GLU 21 2734 3901 -1519 -1565 1123 5203 ATOM 163 C GLU 21 29.159 20.594 48.689 1.000 16.44 ANISOU 163 С GLU 21 1271 2295 2679 -165 -53 430 GLU 21 28.599 19.700 49.329 1.000 14.30 ATOM 164 0 ANISOU 164 0 GLU 21 1271 2257 1907 -417 -301 3 6 165 PHE 22 28.548 21.257 47.708 1.000 16.14 ATOM NPHE ANISOU 165 22 1440 -316 -28 328 N 2441 2253 PHE 20.947 47.327 1.000 15.36 ATOM 166 CA22 27.155 2012 ANISOU 166 CAPHE 22 1530 2294 -262 -173 2 8 1 21.967 46.343 1.000 15.43 ATOM 167 CBPHE 22 26.612 2056 ANISOU 167 CB PHE 22 1863 1944 -316 -247 1 8 4 21.932 46.077 1.000 15.59 MOTA 168 CG PHE 22 25.119 ANISOU 168 CG PHE 22 1822 2141 1962 -299 -170 5 6 1 CD1 PHE 21.987 47.129 1.000 17.03 22 24.218 MOTA 169 ANISOU 169 CD1 PHE 22 2605 1943 -410 -162 - 40 1923 170 CD2 PHE 22 21.856 44.797 1.000 14.84 MOTA 24.606 22 2083 ANISOU 170 CD2 PHE 1541 2013 51 - 94 - 155 ATOM 171 CE1 PHE 22 22.861 21.938 46.906 1.000 15.96 ANISOU 171 CE1 PHE 1805 -159 -64 176 22 1844 2414 MOTA 172 CE2 PHE 22 23.243 21.797 44.551 1.000 15.81 ANISOU 172 CE2 PHE 22 1600 1993 2416 -261 -190 -176 21.853 45.612 1.000 14.18 ATOM 173 CZ PHE 22 22.360 1427 ANISOU 173 CZPHE 22 1430 2531 -105 -164 3 2 5 19.515 46.792 1.000 16.23 ATOM 174 С PHE 22 27.049 ANISOU 174 С PHE 22 -110 164 102 1325 2042 2797 18.751 47.229 1.000 13.24 175 22 MOTA 0 PHE 26.183 ANISOU 175 0 PHE 22 1411 1743 1876 105 -194 3 9 1 23 MOTA 176 N ARG 27.888 19.097 45.853 1.000 15.45 23 ANISOU 176 1971 -167 -80 289 N ARG 1585 2313 17.746 45.325 1.000 15.49 CA ARG ATOM 177 23 27.865 CA ARG ANISOU 177 50 -41 23 809 2443 2634 CB ARG 28.928 17.539 44.248 1.000 17.81 178 ATOM 23 2658 -128 43 -167 ANISOU 178 23 966 3142 CB ARG 179 23 28.470 17.928 42.860 1.000 25.86 MOTA CG ARG 4636 ANISOU 179 CG ARG 23 2719 2470 -758 **-**176 - 49 ATOM 180 CD ARG 23 29.485 17.370 41.867 1.000 34.68 ANISOU 180 CDARG 23 5148 4847 3183 -1532 1634 - 548 ATOM 181 NΕ ARG 23 30.660 18.253 41.877 1.000 31.13 ANISOU 181 ΝE ARG 23 2799 4194 4836 305 747 6 6 23 30.703 182 CZARG 19.424 41.244 1.000 34.24 ATOM ANISOU 182 ARG 23 5418 CZ2749 -757 239 764 4844 MOTA 183 NH1 ARG 23 29.647 19.856 40.551 1.000 28.06 ANISOU 183 NH1 ARG 23 2714 3685 4263 -721 555 181

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ATOM	184	NH2	מ ע	23	31.830	20 114	41 240	1.000 36.08
ANISOU		NH2		23	2261	5328		-562 776 - 8 6
	185	C	ARG	23				1.000 15.06
ANISOU		C	ARG		28.045	16.713		
	186			23	1071	2061		
		0	ARG	23	27.335	15.687		1.000 16.28
ANISOU		0	ARG	23	1443	2244	2497	-118 -71 -277
	187	N	ARG	24	28.952	16.988	47.353	1.000 15.27
ANISOU		N	ARG	24	1024	2156	2623	-52 -21 2 9
	188	CA	ARG	24	29.193	16.003	48.430	1.000 17.70
ANISOU		CA	ARG	24	1443	2589	2693	275 -2 2 1 5
	189	CB	ARG	24	30.466	16.422	49.148	1.000 21.11
ANISOU		CB	ARG	24	1244	3486	3289	484 -257 3 8 4
	190	CG	ARG	24	31.787	16.217	48.429	1.000 30 . 46
ANISOU		CG	ARG	24	1438	5078	5057	426 441 308
	191	CD	ARG	24	32.979	16.537	49.330	1.000 33.50
ANISOU		CD	ARG	24	1163	5831	5736	208 370 458
	192	NE	ARG	24	33.636	17.804	49.071	1.000 51.46
ANISOU		NE	ARG	24	5800	7316	6437	-2596 -1688 1165
	193	CZ	ARG	24	33.973	18.776	49.903	1.000 46.72
ANISOU		CZ	ARG	24	4738	6888	6124	-1719 -1822 1316
	194		ARG	24	33.731	18.728	51.213	1.000 44.24
ANISOU			ARG	24	2650	6998	7160	-392 1001 8 4
	195		ARG	24	34.579	19.871	49.448	1.000 42.82
ANISOU			ARG	24	5339	4428	6503	513 -991 1 2 1 6
	196	C	ARG	24	27.972	15.887	49.334	1.000 17.16
ANISOU		C	ARG	24	1549	2071	2900	129 140 295
	197	0	ARG	24	27.536	14.779		1.000 15.38
ANISOU		0	ARG	24	1706	1890	2247	72 -388 1 0 4
	198	N	CYS	25	27.355	17.011		1.000 12.91
ANISOU ATOM	198	N CA	CYS	25	907 182		76 -25	
ANISOU			CYS	25	26.105			1.000 12.45
ANISOU	200	CA CB	CYS CYS	25	942 183			78 -480 8 1
ANISOU		CB	CYS	25 25	25.660 1150	18.491 1759	1527	1.000 11.67 -136 -604 1 8 4
ATOM	201	SG	CYS	25	23.973	18.580	51.425	1.000 14.90
ANISOU		SG	CYS	25	1465	1593	2602	-164 -26 - 18
ATOM	202	C	CYS	25	25.001			1.000 11.67
ANISOU		Ċ	CYS	25	893 189			33 -64 - 8 6
ATOM	203	Ö	CYS	25	24.360	15.377		1.000 12.73
ANISOU		0	CYS	25	1347	1426	2064	-233 -196 1 2 3
ATOM	204	И	LEU	26	24.798		48.470	1.000 11.70
ANISOU		N	LEU	26	1102	1530	1814	-128 -390 1
ATOM	205	CA	LEU	26	23.766	15.716		1.000 11.11
ANISOU			LEU	26				-238 -79 -194
ATOM	206	СВ	LEU	26	23.674	16.198		1.000 11.54
ANISOU		CB	LEU	26	1345	1522	1518	-75 -84 -202
ATOM	207	ĊĠ	LEU	26	23.242	17.638	46.019	1.000 12.42
ANISOU		ĊĞ	LEU	26	1199	1542	1978	-153 -167 - 40
ATOM	208		LEU	26	23.414	17.993	44.539	1.000 14.77
ANISOU			LEU	26	1428	1916	2270	43 131 4 0 1
ATOM	209		LEU	26	21.814	17.885	46.466	1.000 14.45
ANISOU			LEU	26	1384	2061	2047	264 -32 3 2 1
ATOM	210	C	LEU	26	23.979	14.209		1.000 12.93
ANISOU		Č	LEU	26	1360	1542	2011	-121 -486 - 107
MOTA	211	0	LEU	26	23.011	13.461		1.000 13.78
ANISOU		0	LEU	26	1660	1450	2125	-305 -426 - 51
ATOM	212	N	ARG	27	25.196	13.721		1.000 14.09
ANISOU	212	N	ARG	27	1518	1729	2108	151 -530 - 105
ATOM	213	CA	ARG	27	25.491	12.283		1.000 15.39
ANISOU		CA	ARG	27	2260	1690	1897	186 141 -354
MOTA	214	СB	ARG	27	26.846	12.122		1.000 17.04

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ANTSOU 215 CG ARG 27 3110 2837 3583 1105 606 -399 ANTOM 216 CD ARG 27 2976 3836 4710 1190 720 -1381 ANTSOU 216 CD ARG 27 2976 3836 4710 1190 720 -1381 ANTSOU 217 NE ARG 27 29.818 1.407 47.581 1.000 36.51 ANTSOU 217 NE ARG 27 36.33 4937 5301 121 391 -1429 ANTSOU 218 CZ ARG 27 33.34 5192 5941 364 661 -1.776 ANTSOU 218 CZ ARG 27 33.34 5192 5941 364 661 -1.776 ANTSOU 219 NH1 ARG 27 31.565 12.340 46.401 1.000 48.56 ANTSOU 219 NH2 ARG 27 31.606 12.340 46.401 1.000 40.23 ANTSOU 219 NH2 ARG 27 31.606 12.340 46.401 1.000 40.23 ANTSOU 220 NH2 ARG 27 2891 6127 6266 457 717 -2463 ANTSOU 220 NH2 ARG 27 28.916 12.340 48.949 1.000 14.66 ANTSOU 221 C ARG 27 72.9 1617 2233 135 -33 -42 ATOM 221 C ARG 27 1720 1617 2233 135 -33 -42 ATOM 222 O ARG 27 1981 1533 3114 98 -394 155 ATOM 223 N ASP 28 26.031 12.308 49.973 1.000 17.44 ANTSOU 223 N ASP 28 26.227 11.701 51.277 1.000 15.33 ANTSOU 224 CA ASP 28 1886 1704 224 CA ASP 28 26.227 11.701 51.277 1.000 15.33 ANTSOU 224 CA ASP 28 26.227 11.701 51.277 1.000 15.33 ANTSOU 224 CA ASP 28 27.541 12.280 51.842 1.000 18.31 ANTSOU 225 CB ASP 28 2092 2709 2155 186 -465 54 4 ANTSOU 225 CB ASP 28 28.7541 12.280 51.842 1.000 18.31 ANTSOU 225 CB ASP 28 2002 3883 3176 -96 -50 47 8 ANTSOU 227 OD1 ASP 28 25.15 255 418 38.000 23.06 ANTSOU 227 OD1 ASP 28 28.7541 12.598 51.283 1.000 20.05 ANTSOU 229 C ASP 28 2002 3883 3176 -96 -50 47 8 ANTSOU 229 C ASP 28 2002 3883 3176 -96 -50 47 8 ANTSOU 229 C ASP 28 28.7541 12.598 51.283 1.000 10.05 ANTSOU 229 C ASP 28 28.7541 12.598 51.283 1.000 10.05 ANTSOU 229 C ASP 28 28.7541 12.598 51.283 1.000 10.05 ANTSOU 229 C ASP 28 28.7541 12.598 51.283 1.000 10.05 ANTSOU 229 C ASP 28 28.7541 12.598 51.283 1.000 10.05 ANTSOU 229 C ASP 28 28.7541 12.598 51.284 12.000 18.24 ANTSOU 229 C ASP 28 28.7541 12.598 51.284 12.000 18.24 ANTSOU 229 C ASP 28 28.7541 12.598 51.284 12.000 114.50 ANTSOU 220 C ASP 28 28.754 12.599 51.284 12.599 32.290 32.77 ANTSOU 227 OD1 ASP 28 28.754 12.599 52.267 1.000 12.59 ANTSOU 229 C ASP 28 28.754 12.599 52.267 1.000 12.59 ANTSOU 229 C ASP 28 28.754 12	ANISOU ATOM	215	CG	ARG ARG	27 27	2259 27.502	10.780		517
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                       10.677
                                34.273
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ATOM
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ATOM
ANISOU 311
           CG
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                                               541 -637 -1052
                                28.940 49.910 1.000 28.66
      312
           CD1 LEU
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                        10.472
ATOM
                    39
ANISOU 312
           CD1 LEU
                        3375
                                2293
                                        5221
                                               581 -150 - 190
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           CD2 LEU
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MOTA
      313
                        8.838
ANISOU 313
           CD2 LEU
                    39
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                                        5496
                                               1275 -1485 -208
       314
           С
                                32.430 52.949 1.000 26.26
ATOM
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                    39
                        12.060
           С
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ANISOU 314
               LEU
                    39
                        2868
                                3969
                                        3143
                                31.861 53.266 1.000 35.57
ATOM
      315
           0
               LEU
                    39
                        13.105
ANISOU 315 O
               LEU
                    39
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                                4057
                                        4470
                                               804 -630 3 2 0
       316 N
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MOTA
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4 0
4 0
ANISOU 319
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MOTA
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               THR
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ANISOU 320
                        2646
           CB
               THR
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                                        2874
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            OG1 THR
                                35.687 54.986 1.000 36.24
MOTA
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                    40
                        11.639
                    40
ANISOU 321
            OG1 THR
                        5158
                                3872
                                        4740
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            CG2 THR
                    40
MOTA
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                                34.669 54.659 1.000 34.29
       322
ANISOU 322
            CG2 THR
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ATOM
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ANISOU 323
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MOTA
       324
           CA ASP
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ANISOU 324
           CA ASP 41
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                                        2968
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                        1935
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                                34.785 57.896 1.000 24.69
ATOM
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                ASP 41
                         8.418
ANISOU 325
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                ASP
                    41
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                                 34.846 58.163 1.000 24.79
ATOM
       326
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ANISOU 326
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ANISOU 327
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MOTA
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MOTA
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ATOM
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ANISOU 330
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            OD2 ASP
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MOTA
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MOTA
       332
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ANISOU 332
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           CA
                THR
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                         4852
                                 3472
                                        4475
MOTA
       333
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                THR
                     42
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ANISOU 333
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                THR
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ATOM
       334
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                THR
                     42
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                THR 42
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MOTA
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            OG1 THR 42
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- 101 -ANISOU 336 OG1 THR 42 6998 3682 6912 -3163 -1478 177 337 CG2 THR 42 8.582 39.253 55.872 1.000 45.59 337 CG2 THR 42 9083 3877 4363 -2166 -1048 338 N GLU 43 7.573 35.773 54.862 1.000 31.74 ANISOU 337 -2166 -1048 2 3 8 ATOM N GLU 43 3380 4360 4319 -673 -223 -7 CA GLU 43 6.647 35.355 53.810 1.000 35.40 CA GLU 43 4856 4683 3913 -1510 -860 3 C GLU 43 5.643 34.324 54.330 1.000 28.03 ANISOU 338 N -673 -223 - 782 ATOM 339 ANISOU 339 -1510 -860 3 2 9 34.324 54.330 1.000 28.03 340 C MOTA GLU 43 ANISOU 340 C 2988 3297 4363 -41 -919 1 6 8 341 GLU 43 34.138 53.764 1.000 38.18 ATOM 0 4.560 GLU 43 ANISOU 341 0 3818 2970 7717 -66 -2774 1469 GLU 43 342 CВ ATOM 7.423 34.811 52.608 1.000 38.89 ANISOU 342 СB GLU 43 3779 4464 6532 -2546 -860 - 393 35.745 52.010 1.000 46.47 MOTA 343 CG GLU 43 8.462 ANISOU 343 GLU 43 CG 5175 7105 5377 -2936 -92 -289 9.750 35.764 52.826 1.000 46.40 344 CD GLU MOTA 43 ANISOU 344 CD GLU 7977 -3155 548 -1210 43 4506 5145 345 OE1 GLU ATOM 43 9.775 36.447 53.880 1.000 55.20 ANISOU 345 OE1 GLU 7607 4627 8741 43 -2062 -1002 -669 346 OE2 GLU 43 10.706 35.080 52.433 1.000 56.77 ATOM 4592 8930 8050 -2652 939 -5.980 33.645 55.426 1.000 22.72 ANISOU 346 OE2 GLU 43 -2652 939 -1258 347 LEU ATOM N 44 2508 2161 3964 464 -476 -5.117 32.592 55.959 1.000 26.76 ANISOU 347 Ν LEU 44 464 -476 - 450 MOTA348 CALEU 44 ANISOU 348 1973 4187 140 570 - 986 31.585 56.727 1.000 28.25 CA LEU 444009 CB LEU 5.978 ATOM 349 44 ANISOU 349 5094 CB LEU 2194 -153 277 -562 443448 30.494 57.533 1.000 32.03 ATOM350 CG LEU 5.284 44ANISOU 350 CG LEU 5971 3398 -279 1192 - 627 44 2801 ATOM 351 CD1 LEU 44 4.485 29.535 56.656 1.000 37.95 ANISOU 351 CD1 LEU 44 7665 2239 -1148 2039 - 1403 4514 MOTA 352 CD2 LEU 44 6.302 29.703 58.361 1.000 36.97 ANISOU 352 CD2 LEU 44 7096 2869 4080 1150 2171 1 8 6 ATOM 353 C LEU 44 4.000 33.145 56.841 1.000 31.10 ANISOU 353 C LEU 44 3835 3182 4800 -700 837 -2205 ATOM 354 O LEU 44 2.913 32.543 56.867 1.000 30.19 ATOM 354 O LEU 44 2.913
ANISOU 354 O LEU 44 4402
ATOM 355 N ALA 45 4.238
ANISOU 355 N ALA 45 2897
ATOM 356 CA ALA 45 3.382
ANISOU 356 CA ALA 45 2716
ATOM 357 C ALA 45 1.943
ANISOU 357 C ALA 45 2697 -1248 870 -2165 3299 3768 34.247 57.547 1.000 28.74 2938 5083 -562 710 -2061 34.751 58.623 1.000 27.09 2817 4761 -751 467 -2140 35.014 58.195 1.000 24.95 2697 -784 709 -1257 3673 3110 358 O ALA 45 1.021 MOTA 34.515 58.875 1.000 22.50 ALA 45 2762 ANISOU 358 O 2585 -565 560 -1146 3201 359 CB ALA 45 3.975 MOTA 36.005 59.248 1.000 36.30 ANISOU 359 CB ALA 45 3259 4219 6315 -1912 1332 - 3404 MOTA 360 N SER 46 1.729 35.779 57.128 1.000 26.85 ANISOU 360 N SER 46 3258 3756 3187 -1732 618 -1184 361 36.052 56.642 1.000 24.97 MOTA CA SER 46 0.380 ANISOU 361 CA SER 46 3686 3189 2611 -1223 511 -1105 362 MOTA CB SER 46 0.422 36.950 55.392 1.000 32.35 ANISOU 362 CB SER 46 5428 3395 -2232 70 - 458 3467 ATOM 363 OG SER 46 0.630 38.289 55.772 1.000 45.77 ANISOU 363 OG -2746 2499 - 807 SER 46 7730 3349 6313 MOTA 364 C 46 -0.408 34.787 56.307 1.000 20.63 SER C ANISOU 364 SER 46 2797 2469 2572 -423 -151 - 542 MOTA 365 0 SER 46 -1.578 34.672 56.698 1.000 21.93 ANISOU 365 0 SER 46 3120 2486 2725 -559 305 - 403366 N 33.855 55.590 1.000 22.39 MOTA ALA 47 0.211 ANISOU 366 N 3096 2167 -488 394 - 368 ALA 47 3244

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- 102 -
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ATOM
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ANISOU 367
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MOTA
ANISOU 368
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ANISOU 370
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ANISOU 371
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MOTA
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MOTA
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ANISOU 373
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MOTA
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ATOM
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ANISOU 376
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ATOM
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ATOM
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ANISOU 383
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ANISOU 384
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ANISOU 385
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ANISOU 386
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ATOM
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ATOM
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ATOM
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 ANISOU 391
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 ATOM
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            CD2 LEU
 MOTA
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                     50
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 MOTA
                 VAL
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ANISOU 397 ATOM 398 ANISOU 398	CA VAL CB VAL CB VAL	51 51	3154 -4.281	1763 28.415	1947 56.889	-401 -15 - 427 1.000 16.07 -621 -255 - 501
ATOM 399 ANISOU 399 ATOM 400	CG1 VAL CG1 VAL CG2 VAL	51 51 51 51	2981 -3.002 2959 -5.006	1629 28.114 2382 27.119	1496 57.668 1875 56.497	1.000 18.99 -383 -100 3 0 2 1.000 22.16
ANISOU 400	CG2 VAL	51	4569	2121	1728	-1393 64 - 869
ATOM 401 ANISOU 401	C VAL	51 51	-5.446 2508	28.899 2223	59.114 2009	1.000 17.74 -435 142 -445
ATOM 402	O VAL	51	-6.430	28.187	59.346	1.000 19.76
ANISOU 402 ATOM 403	O VAL N ILE	51 52	3005 -4.671	2160 29.263	2345 60.125	-692 726 -1021 1.000 20.23
ANISOU 403	N ILE	52	2980	29.203	1760	-649 364 -902
ATOM 404 ANISOU 404	CA ILE	52 52	-4.990 3200	28.875	61.507	1.000 20.17
ATOM 405	CB ILE	52 52	-3.847	2665 29.230	1800 62.469	-758 627 -1134 1.000 21.31
ANISOU 405	CB ILE	52	3294	3151	1652	-449 462 -1043
ATOM 406 ANISOU 406	CG2 ILE	52 52	-4.238 3543	29.178 2826	63.931 1719	1.000 21.29 -362 529 -689
ATOM 407	CG1 ILE	52	-2.619	28.346	62.217	1.000 25.37
ANISOU 407 ATOM 408	CG1 ILE	52 52	3213 -2.871	3819 26.872	2608 62.470	-307 727 -1090 1.000 28.56
ANISOU 408	CD1 ILE	52	3474	3578	3798	106 178 -1110
ATOM 409 ANISOU 409	C ILE	52 52	-6.284 3119	29.514 3 21 6	61.950 2190	1.000 22.44 -710 645 -1228
ATOM 410	0 ILE	52	-7.072	28.856	62.647	1.000 23.23
ANISOU 410	O ILE	52	3390	3654	1781 61.530	-766 758 -1246 1.000 23.33
ATOM 411 ANISOU 411	N ASP N ASP	53 53	-6.519 2897	30.754 3064	2903	-626 700 -1361
ATOM 412	CA ASP	53 53	-7.826	31.335	61.897	1.000 24.49 -759 781 -1545
ANISOU 412 ATOM 413	CA ASP CB ASP	53	2818 -7.942	3347 32.781	3141 61.411	1.000 27.43
ANISOU 413	CB ASP	53	2854	3335	4235	-434 819 -1446
ATOM 414 ANISOU 414	CG ASP	53 53	-9.309 3166	33.397 4281	61.570 4326	1.000 30.99 36 1242 -1214
ATOM 415	OD1 ASP	53	-9.657	33.779	62.705	1.000 37.26
ANISOU 415 ATOM 416	OD1 ASP OD2 ASP	53 53	4369 -10.050	4569 33.491	5220 60.553	153 1263 - 2733 1.000 38.45
ANISOU 416	OD2 ASP	53	3393	6043	5173	810 557 -1648
ATOM 417 ANISOU 417	C ASP	53 53	-8.953 3028	30.495 3701	61.316 2634	1.000 24.64 -919 372 -1031
ATOM 418	O ASP	53	-10.011	30.327	61.915	1.000 28.52
ANISOU 418	O ASP N PHE	53 54	3399 -8 744	3835	3603 60 108	-1519 962 -2151 1.000 22.04
ANISOU 419	N PHE	54	2921	2974	2479	-573 174 -704
ATOM 420 ANISOU 420			-9.772 2253	29.187 2879	59.432 2463	1.000 19.99 -421 771 -978
ATOM 421	CB PHE	54	-9.423	29.030	57.942	1.000 18.45
ANISOU 421 ATOM 422			2856 -10 491	1983 3 28.292	2171 57.145	-65 426 -518 1.000 21.36
ANISOU 422	CG PHE	54	3063	2735	2318	-646 599 -627
ATOM 423 ANISOU 423			-11.714 3199	4 28.906 2783	56.933 2826	1.000 23.18 -703 -29 -624
ATOM 424	CD2 PHE	54	-10.29	3 27.035	56.619	1.000 23.32
ANISOU 424 ATOM 425			3482 -12 71	2802 9 28.291	2577 56.241	
ANISOU 425	CE1 PHE	54	3345	3696	3008	-1418 129 - 554
ATOM 426 ANISOU 426			-11.30 3750	3 26.375 3815	55.921 2182	1.000 25.65 -1404 607 -1005
ATOM 42	CZ PHE	5 4	-12.52	2 27.013	55.725	1.000 26.17
ANISOU 42	CZ PHE	54	3433	3830	2679	-1829 298 -813

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27.854 60.132 1.000 19.44
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MOTA
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ANISOU 428
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                                        60.386 1.000 22.11
       429
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                         -11.087 27.450
MOTA
                PHE
                                                -948 1018 -1466
ANISOU 429
           0
                PHE
                     54
                         2601
                                 3066
                                         2734
       430
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                     55
                         -8.882
                                 27.166 60.448 1.000 20.59
MOTA
                PHE
ANISOU 430
           N
                PHE
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                         2728
                                 3375
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                                                -666 180 -611
                                 25.927 61.212 1.000 22.59
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           CA
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                     55
                         -8.966
           CA
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ANISOU 431
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                                 25.360 61.478 1.000 21.93
MOTA
ANISOU 432
           CB
               PHE
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                         3163
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                                         1549
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       433
           CG
                                 24.833 60.284 1.000 20.60
ATOM
               PHE
                         -6.790
ANISOU 433
               PHE
                                         1793
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                         3034
                                 2998
                                                -1004 365 - 375
MOTA
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           CD1 PHE
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                         -7.352
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           CD1 PHE
ANISOU 434
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                         2300
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                                         1717
                                                -1078586 - 271
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            CD2 PHE
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                         -5.430
ANISOU 435
            CD2 PHE
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                                         1241
                                                 -926 128 -497
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ATOM
       436
            CE1 PHE
                     55
                         -6.609
                                 24.037
            CE1 PHE
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ANISOU 436
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ATOM
ANISOU 437
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ATOM
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            C
                PHE
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                         -9.684
                                 26.111 62.546 1.000 24.99
MOTA
ANISOU 439
            С
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MOTA
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ANISOU 440
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                PHE
                     55
                         3802
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                     56
MOTA
       441
            Ν
                GLU
                         -9.330
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ANISOU 441
            Ν
                GLU
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                         2864
                                 4109
                                         2013
                                                 -634 937 -525
                                         64.636 1.000 30.01
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MOTA
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ANISOU 442
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                GLU
                     56
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                                  5378
                                         2394
                                                 -1050 1465 - 994
                                 28.333 65.436 1.000 36.40
MOTA
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            CB
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ANISOU 443
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ATOM
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            CG
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ANISOU 444
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ATOM
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ANISOU 445
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                GLU
                                         3202
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                     56
                         6081
                                  9310
ATOM
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            OE1 GLU
                     56
                         -5.694
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ANISOU 446
            OE1 GLU
                     56
                                                 -3208 -2335 266
                         8034
                                  12274
                                         2769
                                 30.084 66.614 1.000 58.51
       447
            OE2 GLU
                     56
ATOM
                         -7.145
ANISOU 447
                     56
                                                 -2088 1096 - 3951
            OE2 GLU
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                                  9338
                                         4151
                     56
MOTA
       448
            С
                GLU
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                         3764
ANISOU 448
            C
                GLU
                     56
                                  4923
                                         2941
                                                 -977 1967 - 1271
                         -12.058 27.542 65.504 1.000 35.21
MOTA
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            0
                GLU
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ANISOU 449
            0
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                GLU
MOTA
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            N
                HIS
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                HIS
                      57
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MOTA
       451
            CA
                HIS
                     57
                                                 -519
ANISOU 451
            CA
                HIS
                     57
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                          3853
ATOM
       452
                HIS
                     57
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ANISOU 452
            CB
                HIS
                      57
                          3844
                                  5183
                                          3664
ATOM
       453
                      57
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                HIS
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ANISOU 453
            CG
               HIS
                     57
                          4497
                                 5409
                                          3444
MOTA
       454
            CD2 HIS
                          -10.361 31.946 65.071 1.000 35.26
                     57
                                                 -834 637 -1456
ANISOU 454
                                  5214
            CD2 HIS
                      57
                          4837
                                          3345
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ATOM
       455
            ND1 HIS
                      57
            ND1 HIS
ANISOU 455
                      57
                          6021
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                                  5885
 ATOM
        456
            CE1 HIS
                      57
                          -10.798 31.410 67.151 1.000 42.28
 ANISOU 456
                                                  -1632 1099 - 1772
             CE1 HIS
                      57
                          6680
                                  6066
                                          3320
 ATOM
        457
            NE2 HIS
                      57
                          -9.902
                                  31.970 66.362 1.000 41.69
 ANISOU 457
            NE2 HIS
                      57
                          6377
                                  6133
                                          3329
                                                  -1817 407 -1148
                      57
                          -13.769 29.466 62.547 1.000 32.58
 MOTA
        458
             C
                 HIS
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ANISOU	458	С	HIS	57	3083	5097	4199	-729	1723	- 2 () 6	6
MOTA	459	0	HIS	57	-14.902		62.578					
ANISOU			HIS	57	3121	5097	4625		1865		5 6	5
ATOM	460	Й	GLY	58	-13.370		61.432	1.000	28. 1341		= 0	_
ANISOU ATOM	461	N CA	GLY GLY	58 58	2841 -14.326	4353	3742 60.332	-253 1.000			5 U	0
ANISOU		CA	GLY	58	2471	3916	3869	24 129		117	3	
ATOM	462	C	GLY	58	-15.447		60.738	1.000			_	
ANISOU	462	С	GLY	58	2665	4357	4353		1323		0 5	8
MOTA	463	0	GLY	58	-15.241		61.534	1.000				
ANISOU		0	GLY	58	2976	4044	4087		1192		2 9	7
ATOM ANISOU	464 464	N	SER SER	59 59	-16.635 2556	27.958 3905	60.193 4029	1.000	27.6 1461		76	7
ATOM	465	CA	SER	59	-17.812		60.497	1.000			10	1
ANISOU		CA	SER	59	2675	4074	4049		1294		3 2	5
ATOM	466	СВ	SER	59	-19.121		60.162	1.000	28.2	2 9		
ANISOU	466	CB	SER	59	2556	4574	3618		1198		2 8	}
MOTA	467	OG	SER	59	-19.229		58.739	1.000				
ANISOU		OG	SER	59	3598	3742	3547		1729		6 7	1
ATOM ANISOU	468	C	SER SER	59 59	-17.795 3467		59.724	1.000 -646	29.: 1463		2 0	. 6
ANISOU	469	0	SER	5 9 5 9	-16.990	3990 25 651	3779 58.810	1.000			20	. 0
ANISOU		Ö	SER	59	3054	3042	2537		648		6 9	9
ATOM	470	N	GLU	60	-18.698		60.103	1.000				
ANISOU	470	N	GLU	60	2413	3900	3907		1079		5 3	3
ATOM	471	CA	GLU	60		23.684		1.000				
ANISOU		CA	GLU	60	2699	3515	4037	-98	709		3 7	7
ATOM ANISOU	472	CB CB	GLU GLU	60	-19.646 5393	4393	60.001 5075	1.000 -1361			1	
ATOM	473	CG	GLU	60 60	-19.011		60.917	1.000			4	
ANISOU		CG	GLU	60	5606	5473	5878	-977	1079		1 9	9
ATOM	474	CD	GLU	60	-17.507		60.797	1.000				
ANISOU	474	CD	GLU	60	5714	6217	6503	-390	1207		7	
ATOM	475		GLU	60	-17.030		59.684	1.000	48.	11	_	_
ANISOU			GLU	60	5349	7545	5384	709	366		5	1
ATOM ANISOU	476		GLU GLU	60 60		21.763 5742	61.829	1.000 1158	46. 1550		5 (٦ /
ANISOU	477	C C	GLU	60 60	4926 -19 091	23.960	7000 57.915	1.000			5 (<i>)</i> -±
ANISOU		Č	GLU	60	2829	2728	4055	86 725				
ATOM	478	Ō	GLU	60		23.346		1.000				
ANISOU		0	GLU	60	2119	2980	4091	-202	741	- 7	5	2
MOTA	479	N	ALA	61		24.890		1.000				_
ANISOU		N	ALA	61	2083	3206	4432	-34	612	- 7	7	4
ATOM ANISOU	480	CA CA	ALA	61			56.368	1.000 228		U 5 1	0	5 5
ATOM	481	CB	ALA ALA	61 61	1838 -21 670	2999 26.176	4301 56.459	1.000				ر ر
ANISOU		CB	ALA	61	2807	1857	5797	394	704		0	6
ATOM	482	Č	ALA	61		5 25.790	55.500	1.000	27.	31		
ANISOU		C	ALA	61	3170	2572	4633	-377	1178		. 0	2 6
ATOM	483	0	ALA	61		7 25.467	54.311	1.000				
ANISOU		0	ALA	61	2363	1876	4232	42 66				
ATOM ANISOU	484	N	GLU GLU	62 62	2075	26.642 2258	56.118 4094	1.000 396	569		۹ ۶	4
ATOM	485	CA	GLU	62		2230 5 27.258					, ,	-
ANISOU		CA	GLU	62	2401	2603	4188	150	852	5	5 9	0
ATOM	486	СВ	GLU	62		6 28.354				68		
ANISOU		СВ	GLU	62	2401	2490	4485	91 12	73 -	- 82	8	
ATOM	487	CG	GLU	62		1 29.636						_
ANISOU		CG	GLU	62	2542	2620	4409	353	421		5 S	כ
ATOM ANISOU	488	CD	GLU GLU	62 62		8 30.581 2991		1.000		. 2 /	1 2	Q.
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\mathtt{ATOM}	489	OE1	GLU	62	-16.527	30 241	58.410	1.000 30.11
ANISOU	489		GLU	62	3231	3067	5143	
ATOM	490		GLU	62	-17.796	31 730	5145	318 56 - 1639
ANISOU			GLU	62	4832	31./39	5/.436	1.000 35.30
ATOM	491	C				2994	5584	863 109 -1327
ANISOU			GLU	62	-16.409		55.025	1.000 21.70
		C	GLU	62	2394	2421	3430	30 784 - 579
ATOM	492	0	GLU	62	-15.818	26.218	53.940	1.000 19.44
ANISOU		0	GLU	62	2095	2140	3153	-301 467 -604
ATOM	493	N	LYS	63	-16.184		55.972	1.000 20.08
ANISOU	493	N	LYS	63	2472	2266	2893	
ATOM	494	CA	LYS	63	-15.246			-74 761 - 902
ANISOU		CA	LYS	63	2322		55.678	1.000 19.73
ATOM	495	CB	LYS	63		2559	2614	133 429 - 903
ANISOU		CB			-14.934			1.000 18.48
ATOM	496		LYS	63	1803	2743	2476	-218 587 - 836
		CG	LYS	63	-13.946	24.240	57.881	1.000 19.17
ANISOU		CG	LYS	63	2115	2332	2836	-296 325 -674
ATOM	497	CD	LYS	63	-13.839	23.651	59.290	1.000 26.23
ANISOU		CD	LYS	63	2978	4084	2902	-888 -177 - 287
ATOM	498	СE	LYS	63	-12.753		60.068	1.000 27.75
ANISOU	498	CE	LYS	63	3074	5008	2461	-1239 500 -1082
ATOM	499	NZ	LYS	63	-12.929	24 270		
ANISOU	499	ΝZ	LYS	63	3177		61.530	1.000 34.95
ATOM	500	C	LYS			7579	2524	-2594 840 - 894
ANISOU		C		63	-15.789	23.304		1.000 17.52
ATOM			LYS	63	2014	2191	2453	51 529 - 691
_	501	0	LYS	63	-15.025		53.654	1.000 17.58
ANISOU		0	LYS	63	2266	1709	2704	158 707 -653
ATOM	502	N	ARG	64	-17.069	22.912	54.641	1.000 19.63
ANISOU		N	ARG	64	2081	2452	2926	-14 614 -592
ATOM	503	CA	ARG	64	-17.618		53.595	1.000 19.00
ANISOU	503	CA	ARG	64	1509	2526	3185	-3 620 - 652
ATOM	504	С	ARG	64	-17.471	22 634	52 104	1.000 20.42
ANISOU	504	С	ARG	64	2165	2436	3157	
ATOM	505	0	ARG	64	-17.204			-390 -22 -536
ANISOU		Ö	ARG	64	1854		51.195	1.000 18.83
ATOM	506	СB	ARG	64		2184	3115	-434 575 -201
ANISOU		CB	ARG	64	-19.080	21.6/0	53.871	1.000 24.70
ATOM	507	CG			1470	3652	4263	-51 841 -909
ANISOU			ARG	64	-19.838		52.795	1.000 36.49
ATOM		CG	ARG	64		5284	5621	-2020 138 -882
	508	CD	ARG	64	-21.315		53.095	1.000 46.32
ANISOU		CD	ARG	64	3034	6962	7603	-2438 327 -1187
ATOM	509	NE	ARG	64	-21.776	21.216	54.331	1.000 55.81
ANISOU		NE	ARG	64	3917	8636	8652	-396022222 - 1870
MOTA	510	CZ	ARG	64	-22.814	21.840	54.811	1.000 58.82
ANISOU		СZ	ARG	64	4438	8939	8972	-3479 1988 -2480
ATOM	511	NH1	ARG	64	-23.884			1.000 76.83
ANISOU	511	NH1	ARG	64	6024	9527	13641	-1787 -165 -1872
ATOM	512	NH2		64	-22.797		56.093	
ANISOU	512	NH2		64		9201		1.000 69.53
ATOM	513	N	ALA	65	-17.621		9424	-5884 3891 -3304
ANISOU		N	ALA	65			52.066	1.000 20.43
ATOM	514	CA	ALA			2554	3519	24 612 - 5 2 5
ANISOU		CA		65	-17.505		50.782	1.000 19.45
ATOM	515		ALA	65	1649	2216	3523	409 184 - 553
ANISOU		CB	ALA	65	-17.912	26.108	50.984	1.000 23.73
		CB	ALA	65	1420	2019	5579	126 -373 - 742
ATOM	516	C	ALA	65	-16.118	24.549	50.168	1.000 17.89
ANISOU		С	ALA	65	1524	2099	3173	-47 108 -101
ATOM	517	0	ALA	65	-15.983	24.732	48.954	1.000 18.77
ANISOU		0	ALA	65		2178	3123	122 -8 - 229
ATOM	518	N	VAL	66	-15.100	24.248	50.973	1.000 17.99
ANISOU	518	N	VAL	66		2151	3137	-86 36 -196
MOTA	519	CA	VAL	66	-13.746			1.000 16.74
				-		_ 1.000	20.420	1.000 10.74

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ANISOU 519 CAVAL 66 1553 1359 2948 -62 -56 -254 520 CB VAL 66 -12.775 25.151 50.951 1.000 17.29 ANISOU 520 CB VAL 66 1805 1804 2963 -330 338 -185 521 CG1 VAL 66 ATOM -13.238 26.532 50.455 1.000 16.70 CG1 VAL ANISOU 521 66 1547 1800 2997 545 - 553 111 CG2 VAL 66 -12.652 25.180 52.462 1.000 18.65 MOTA 522 1996 ANISOU 522 CG2 VAL 66 2053 3036 -193 17 - 538 523 MOTA VAL 66 -13.201 22.680 50.724 1.000 15.66 ANISOU 523 VAL 66 1775 1813 2362 -70 -250 - 457 MOTA 524 0 VAL 66 -11.972 22.493 50.808 1.000 14.19 ANISOU 524 0 VAL 66 1747 1576 2069 -122 -56 -347525 THR -14.071 21.695 ATOM 67 50.873 1.000 14.46 N ANISOU 525 THR 67 N 1550 2343 1602 126 -48 -722 MOTA 526 CATHR 67 -13.723 20.279 51.000 1.000 14.06 ANISOU 526 CATHR 67 1461 1698 2185 234 5 - 740 527 СВ 67 MOTA THR -14.419 19.647 52.225 1.000 15.08 ANISOU 527 CB THR 67 1721 1955 2053 -51 -426 - 444 ATOM 528 OG1 THR 67 -14.089 20.337 53.453 1.000 17.41 ANISOU 528 67 OG1 THR 2538 1949 2128 -39 70 - 716 529 CG2 THR 67 -13.915 18.215 52.420 1.000 16.63 MOTA CG2 THR ANISOU 529 67 2182 148 293 -658 1888 2248 67 MOTA 530 С THR -14.067 19.518 49.728 1.000 12.37 67 ANISOU 530 C THR 1144 1422 2132 209 -95 -517 67 MOTA 531 0 THR -15.208 19.567 49.229 1.000 14.82 ANISOU 531 0 THR 67 1197 2086 2350 208 -168 - 362 ATOM 532 Ν SER 68 -13.092 18.790 49.180 1.000 11.61 ANISOU 532 1109 37 - 58 - 534 NSER 68 1421 1881 533 CASER -13.306 17.955 48.003 1.000 11.45 ATOM 68 ANISOU 533 CA SER 68 1274 1444 1631 -49 -30 -374 ATOM 534 CB -12.027 17.317 47.480 1.000 11.88 SER 68 ANISOU 534 79 252 - 157 CB SER 68 1446 1523 1544 MOTA 535 -11.026 18.292 47.239 1.000 16.95 OG SER 68 ANISOU 535 OG SER 68 1557 2314 2569 -336 389 -218 ATOM С -14.269 16.815 48.319 1.000 11.56 536 SER 68 ANISOU 536 C SER 68 1287 1375 1732 -61 53 - 406 537 ATOM 0 SER 68 -14.308 16.384 49.476 1.000 14.62 ANISOU 537 0 SER 68 1998 1860 1697 -538 153 -430 69 MOTA 538 N PRO -15.026 16.324 47.344 1.000 12.78 ANISOU 538 69 -243 -88 -194 Ν PRO 1476 1473 1905 69 69 ATOM 539 CD PRO -15.130 16.801 45.953 1.000 12.47 PRO ANISOU 539 CD 1808 1909 -199 -203 - 144 1022 PRO 540 69 MOTA CA -15.941 15.214 47.639 1.000 12.21 ANISOU 540 PRO 69 CA1358 1369 1913 -178 148 -437 PRO 69 MOTA 541 CB -16.825 15.193 46.355 1.000 13.94 ANISOU 541 69 CB PRO 1362 1591 2343 -251 -178 - 14 69 MOTA 542 CG PRO -15.924 15.715 45.290 1.000 14.38 1396 ANISOU 542 CG PRO 69 1947 2122 -554 -511 1 7 8 -15.270 13.882 47.912 1.000 13.25 MOTA 543 C PRO 69 ANISOU 543 PRO 69 1206 2303 -217 -115 - 100 1526 544 MOTA 0 PRO 69 -15.932 12.985 48.481 1.000 14.01 ANISOU 544 0 PRO 69 1753 1450 2122 -373 99 - 301 545 ATOM NVAL 70 -14.015 13.692 47.554 1.000 13.46 ANISOU 545 VAL N 70 1288 1479 2348 -174 -108 - 265 MOTA 546 CA VAL 70 -13.184 12.548 47.898 1.000 13.49 ANISOU 546 2030 CA VAL 70 1404 1692 37 138 - 195 ATOM 547 CB VAL 70 -12.587 11.720 46.737 1.000 16.39 ANISOU 547 CB 70 -225 614 -452 VAL 2142 1648 2439 CG1 VAL -13.615 10.756 46.208 1.000 33.50 ATOM 548 70 ANISOU 548 70 -2702 41 -867 CG1 VAL 6470 2984 3274 -11.995 12.613 45.640 1.000 16.46 CG2 VAL MOTA 549 70 ANISOU 549 CG2 VAL 70 1749 2234 2273 269 444 2 3

- 108 -VAL 70 -12.042 13.057 48.782 1.000 13.59 VAL 70 1618 1382 2163 -38 -114 1 VAL 70 -11.426 14.105 48.493 1.000 14.20 MOTA 550 C ANISOU 550 C MOTA 551 0 -11.426 14.105 48.493 1.000 14.20 VAL 70 ANISOU 551 0 1748 1685 1964 -265 26 182 PRO 71 MOTA 552 -11.786 12.365 49.898 1.000 14.21 PRO 71 ANISOU 552 1607 1507 2285 -115 -62 310 ATOM 553 CD PRO 71 -12.432 11.125 50.378 1.000 14.70 ANISOU 553 CD PRO 71 1920 1590 2076 -201 646 4 ATOM 554 CA PRO 71 -10.830 12.919 50.878 1.000 17.41 ANISOU 554 CA PRO 71 2429 2008 2178 -522 -342 4 1 8 ATOM 555 CB PRO 71 -11.338 12.304 52.193 1.000 20.87 ANISOU 555 CB PRO 71 3768 2082 -743 190 1 4 2081 MOTA 556 CG PRO 71 -11.908 10.989 51.775 1.000 18.28 ANISOU 556 CG PRO 71 3534 1665 1746 -338 781 -54 C PRO 71
C PRO 71
O PRO 71
O PRO 71
N THR 72
N THR 72
CA THR 72
CA THR 72
CB THR 72 ATOM 557 С PRO 71 -9.384 12.543 50.619 1.000 17.14 ANISOU 557 2183 2304 2026 -684 -815 4 4 MOTA 558 -8.730 11.796 51.330 1.000 20.54 ANISOU 558 2745 2610 2448 -87 -404 4 1 4 ATOM 559 -8.834 13.111 49.556 1.000 16.59 ANISOU 559 2156 2046 -235 -508 - 17 2103 MOTA 560 -7.496 12.818 49.090 1.000 17.43 ANISOU 560 2113 1884 2626 -254 -510 - 288 ATOM 561 -7.477 12.829 47.545 1.000 15.98 72 ANISOU 561 CB THR 1700 1761 2611 211 -458 - 421 72 ATOM 562 OG1 THR -8.027 14.094 47.128 1.000 17.28 ANISOU 562 72 OG1 THR 2146 1553 2868 27 - 355 - 271 CG2 THR ATOM 563 72 -8.348 11.764 46.929 1.000 12.63 CG2 THR ANISOU 563 72 1296 1581 1923 -46 328 --6.418 13.805 49.549 1.000 17.83 1296 328 - 127 ATOM 564 C 72 THR ANISOU 564 C 72 THR 2153 1773 72 2153 1773 2847 -155 -1228 72 -5.216 13.536 49.329 1.000 20.17 2847 -155 -1228 2 3 2 MOTA 565 O THR ANISOU 565 O THR 72 2142 2265 3257 -225 -1049 480 73 -6.785 14.920 50.169 1.000 19.43 73 2876 2052 2455 -782 -451 -ATOM 566 N MET ANISOU 566 N MET -782 -451 -144 73 -5.799 15.944 50.521 1.000 18.75 ATOM 567 CA MET ANISOU 567 CA MET 73 2117 2326 2682 -538 - 466 - 280ATOM 568 СВ MET 73 -4.758 15.338 51.480 1.000 22.03 ANISOU 568 CB MET 73 1826 2825 3718 -377 -306 5 9 5 ATOM 569 73 -5.374 15.059 52.843 1.000 27.01 CG MET ANISOU 569 CG MET 73 3545 2853 -84 -87 1526 3864 ATOM 570 SD 73 -4.107 14.850 54.107 1.000 32.23 MET ANISOU 570 SD MET 73 4364 4245 3637 469 -400 5 8 3 ATOM 571 CE MET 73 -3.179 13.492 53.374 1.000 26.74 ANISOU 571 CE MET 73 2885 4895 2381 326 425 1348 MOTA 572 MET 73 -5.066 16.582 49.355 1.000 17.20 ANISOU 572 С MET 73 1338 2129 3067 -20 -269 - 175 ATOM 573 0 MET 73 -3.945 17.110 49.498 1.000 21.20 ANISOU 573 0 MET 73 1713 2512 3832 -541 51 -1024 574 N ATOM ARG 74 -5.630 16.600 48.175 1.000 18.64 ANISOU 574 N 1881 ARG 74 2051 3150 84 - 461 543 575 CA ARG -5.091 74 17.180 46.967 1.000 15.73 ANISOU 575 CA ARG 74 937 1986 3053 169 27 - 174 ATOM 576 CВ ARG 74 -5.655 16.537 45.704 1.000 16.53 ANISOU 576 CВ ARG 74 1711 1434 3137 -263 142 -160 ATOM 577 CG ARG 74 -4.911 16.934 44.440 1.000 15.01 ANISOU 577 CG ARG 74 1270 1288 3144 -156 279 -554 MOTA 578 CDARG 74 -5.683 16.543 43.185 1.000 16.10 ANISOU 578 CD ARG 74 1967 1031 3120 268 -92 -407 ATOM 579 NEARG 74 -4.902 16.816 41.966 1.000 18.81 ANISOU 579 ΝE ARG 74 2259 1813 3075 -432 -252 - 296 ATOM 580 CZARG 74 -5.033 17.824 41.130 1.000 16.64

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ANISOU 580 CZ ARG 74 1646 2709 -141 -190 - 596 1968 NH1 ARG -5.951 18.775 41.293 1.000 20.09 MOTA 581 74 ANISOU 581 74 1899 2075 NH1 ARG 3660 54 - 353 - 788 582 NH2 ARG 74 -4.22017.896 40.068 1.000 20.12 ANISOU 582 NH2 ARG 74 2366 2844 2437 153 -196 - 400 18.681 46.966 1.000 12.70 ATOM 583 C ARG 74 -5.373ANISOU 583 C ARG 1880 1758 6 - 22 - 13674 1187 MOTA 584 0 ARG 74 -4.50119.465 46.582 1.000 14.07 ANISOU 584 0 ARG 74 1049 2048 2247 -221 -170 -480585 N 75 -6.567 19.099 47.387 1.000 12.72 MOTA ARG ANISOU 585 Ñ ARG 75 1402 1702 1728 95 182 - 108 ATOM 586 CAARG 75 -7.00620.471 47.308 1.000 13.40 ANISOU 586 CAARG 75 1924 1618 1548 87 275 - 193 587 MOTA CВ ARG 75 -7.73720.784 45.995 1.000 13.45 ANISOU 587 CB 75 1387 ARG 1972 1751 -179 51 -588 75 20.637 44.721 1.000 13.38 MOTA CG ARG -6.908 75 ANISOU 588 1594 78 -217 101 СG ARG 1638 1851 -5.849 589 CDARG 75 21.708 44.582 1.000 12.85 ATOM ANISOU 589 CDARG 75 1537 1602 1741 237 62 - 15 590 21.685 43.347 1.000 13.71 ATOM NE ARG 75 -5.087 ANISOU 590 NΕ ARG 75 1708 1797 1705 188 90 - 91 591 75 ATOM CZARG -3.98421.036 43.013 1.000 12.46 ANISOU 591 1731 CZ ARG 75 1348 1656 -89 86 1 1 7 592 75 20.241 43.894 1.000 14.64 MOTA NH1 ARG -3.418 1834 ANISOU 592 NH1 ARG 75 1933 1794 186 -91 6 5 75 ATOM 593 NH2 ARG -3.444 21.167 41.794 1.000 13.72 ANISOU 593 NH2 ARG 75 1510 2037 1667 -136 84 - 83 20.787 48.475 1.000 12.74 ATOM 594 C ARG 75 -7.948-209 214 -464 ANISOU 594 С 75 ARG 1400 1656 1784 19.944 48.818 1.000 14.60 MOTA 595 0 ARG 75 -8.780 ANISOU 595 75 -427 156 -480 0 1926 2273 ARG 1348 76 21.955 49.078 1.000 11.92 596 GLY -7.830 MOTA N ANISOU 596 76 1537 1724 -22 34 - 389 N GLY 1268 CA ATOM 597 GLY 76 -8.801 22.395 50.070 1.000 12.44 1796 ANISOU 597 76 1493 -315 263 -412 CA GLY 1439 MOTA 598 С 76 -8.536 21.857 51.469 1.000 12.50 GLYANISOU 598 C GLY 76 1324 1527 1900 5 326 - 273 599 -7.388 21.517 51.769 1.000 14.25 MOTA 0 GLY 76 ANISOU 599 0 76 2099 2218 -277 239 -225GLY1100 -9.574 21.840 52.287 1.000 12.65 MOTA 600 N PHE 77 ANISOU 600 NPHE 77 1191 1806 1809 -162 231 -351 77 ATOM 601 CA PHE -9.526 21.474 53.694 1.000 14.00 ANISOU 601 PHE 77 -260 276 -138 CA 1295 2110 1914 MOTA 602 PHE 77 -10.644 22.226 54.451 1.000 14.73 CB ANISOU 602 CB PHE 77 1554 2169 1874 -402 485 77 MOTA 603 CG PHE -10.773 21.824 55.912 1.000 17.13 PHE -374 378 -243ANISOU 603 CG 77 1927 2730 1849 CD1 PHE 77 -9.949 22.369 56.886 1.000 19.49 MOTA 604 ANISOU 604 77 2700 -119 219 -789 CD1 PHE 2744 1962 CD2 PHE MOTA 605 77 -11.730 20.902 56.309 1.000 19.13 ANISOU 605 CD2 PHE 77 -501 864 -165 2348 3068 1852 MOTA 606 CE1 PHE 77 -10.068 21.973 58.217 1.000 19.75 -174 -313 - 304 ANISOU 606 CE1 PHE 77 2956 2381 2168 MOTA 607 CE2 PHE 77 -11.829 20.479 57.627 1.000 18.73 ANISOU 607 -382 310 -7777 CE2 PHE 2565 2711 1841 ATOM 608 CZPHE 77 -10.986 21.013 58.584 1.000 19.22 CZANISOU 608 98 13 - 364 PHE 77 2378 2542 2382 609 -9.668 19.976 53.924 1.000 13.73 MOTA C PHE 77 ANISOU 609 C PHE 77 1306 2096 1813 -368 21 - 204 77 MOTA 610 0 PHE -10.520 19.313 53.291 1.000 16.02 ANISOU 610 0 PHE 77 1386 2508 2194 -470 -128 -425

- 110 -THR 78 -8.869 19.439 54.852 1.000 14.33 N ANISOU 611 THR 78 1543 2270 N1629 -472 35 - 49612 CA THR 78 -9.034 18.053 55.276 1.000 15.80 ANISOU 612 CATHR 78 1813 2310 1880 -508 -23 8 2 MOTA 613 THR СВ 78 -8.001 17.081 54.666 1.000 18.26 ANISOU 613 CB THR 78 1583 2199 3158 -599 334 131 OG1 THR ATOM 614 78 -7.924 17.323 53.266 1.000 21.81 OG1 THR ANISOU 614 78 3351 1877 3057 -88 943 - 370 615 CG2 THR 78 -8.419 15.634 54.888 1.000 20.35 ATOM ANISOU 615 CG2 THR 78 2855 2254 2622 -1119 1108 - 707 -8.832 17.881 56.777 1.000 19.14 MOTA 616 THR 78 С ANISOU 616 THR 78 2845 2479 1948 -1747 - 471 1 6 9617 -7.801 18.311 57.290 1.000 22.04 THR 78 MOTA 0 ANISOU 617 THR 78 0 2781 2889 2704 -1718 -985 7 6 3 79 618 GLY ATOM N -9.730 17.203 57.484 1.000 19.20 79 2629 ANISOU 618 GLY 2823 N1844 -1352 19 4 5 79 ATOM 619 CA GLY -9.429 16.695 58.819 1.000 16.69 ANISOU 619 CA GLY 79 1800 2770 -518 196 - 95 1771 -8.672 15.376 58.720 1.000 22.98 79 ATOM 620 GLY С 79 2381 ANISOU 620 GLY2874 3477 -272 -289 -54579 -9.227 14.504 58.044 1.000 25.57 621 0 GLY ATOM79 3683 ANISOU 621 0 GLY 2520 -456 -974 - 141 3514 7.494 80 2412 80 -6 C 622 LEU 80 -7.494 15.236 59.319 1.000 22.91 ATOM N ANISOU 622 N LEU 2900 30 - 206 - 606 3392 LEU -6.644 14.081 59.072 1.000 25.08 623 CAATOM ANISOU 623 CALEU 80 2848 2777 3904 206 621 361 80 80 MOTA 624 C LEU -6.372 13.294 60.370 1.000 24.30 С 2834 ANISOU 624 LEU 2762 3637 -300 480 200 80 625 0 -5.729 MOTA LEU 13.812 61.291 1.000 25.14 80 ANISOU 625 2253 0 LEU 4283 27 145 - 5 3017 626 CB LEU 8 0 MOTA -5.318 14.480 58.415 1.000 27.16 ANISOU 626 CB LEU 80 3057 3326 3937 379 918 641 ATOM 627 CG LEU 8.0 -4.411 13.338 57.933 1.000 29.43 8.0 1260 1 7 3 ANISOU 627 CG LEU 3474 3505 4204 287 CD1 LEU 80 MOTA 628 -5.145 12.438 56.956 1.000 38.31 ANISOU 628 CD1 LEU 80 5673 4993 3891 -1554 1987 - 287 629 CD2 LEU 80 MOTA -3.137 13.884 57.306 1.000 29.85 ANISOU 629 CD2 LEU 80 3502 3919 3920 125 1307 - 264 GLU 81 630 MOTA N -6.853 12.055 60.396 1.000 25.58 ANISOU 630 GLU 81 2469 2759 -196 -82 510 N 4490 CA GLU 81 -6.739 CA GLU 81 2739 C GLU 81 -5.299 C GLU 81 2870 O GLU 81 -4.489 O GLU 81 3709 MOTA 631 -6.739 11.038 61.415 1.000 25.98 -258 -55 424 ANISOU 631 2692 4441 MOTA 632 -5.299 10.536 61.562 1.000 26.28 ANISOU 632 3268 3848 187 407 MOTA 633 -4.489 10.655 60.655 1.000 28.19 ANISOU 633 799 - 544 3520 3483 253 81 CB GLU 61.123 1.000 29.83 ATOM 634 -7.685 9.861 CB GLU 81 ANISOU 634 3533 2894 4906 -770 270 181 CG GLU 81 MOTA 635 -7.241 8.832 60.098 1.000 25.34 ANISOU 635 GLU 81 1737 CG 2915 4976 284 -1220 158 MOTA 636 CD GLU 81 -7.568 9.156 58.649 1.000 27.00 ANISOU 636 CD GLU 81 1841 3405 5012 475 -1887 -456 MOTA 637 OE1 GLU 81 -8.120 10.240 58.324 1.000 28.81 ANISOU 637 -155 7 9 1 OE1 GLU 81 3444 3091 4413 322 ATOM 638 OE2 GLU -7.240 8.273 57.814 1.000 31.31 81 ANISOU 638 OE2 GLU 81 3514 3384 4999 162 352 100 82 MOTA639 N SER -4.988 9.974 62.720 1.000 31.00 ANISOU 639 3780 4430 N SER 82 3568 -65 -30 1484 MOTA 640 CA SER 82 -3.653 9.422 62.959 1.000 30.29 ANISOU 640 CASER 82 3278 3692 4540 -157 -515 1011 MOTA 641 С SER 82 -3.421 8.150 62.150 1.000 31.76

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ANISOU	641	С	SER	82	3995	3241	4831	-102 -1104 8 4 7
ATOM	642	Õ	SER	82	-4.313	7.728	61.397	1.000 34.01
ANISOU		Ö	SER	82	3193			
ATOM	643					3794	5935	458 -1188 1 3 4
		CB	SER	82	-3.463	9.167	64.452	1.000 34.74
ANISOU		CB	SER	82	4687	3907	4606	-232 -979 9 7 1
ATOM	644	OG	SER	82	-2.360	8.305	64.681	1.000 41.53
ANISOU	644	OG	SER	82	4922	5366	5490	236 -1958 9 7 0
ATOM	645	N	GLY	91	-17.230		70.136	1.000 42.64
ANISOU		N	GLY	91	4516	7599	4086	
ATOM	646	CA	GLY	91	-17.485			-2166 2340 - 427
ANISOU		CA					69.789	1.000 44.91
			GLY	91	6666	7702	2697	-4311 -1561 565
ATOM	647	C	GLY	91	-16.227		69.452	1.000 38.67
ANISOU		C	GLY	91	5455	7587	1652	-2821 -274 - 159
ATOM	648	0	GLY	91	-15.164	11.480	70.040	1.000 32.45
ANISOU	648	0	GLY	91	4241	4474	3616	-183 1152 - 439
ATOM	649	N	GLY	92	-16.332	12.558	68.474	1.000 31.97
ANISOU	649	N	GLY	92	3881	5904	2363	-1382 735 -571
ATOM	650	CA	GLY	92	-15.232		68.075	
ANISOU		CA	GLY	92	4121			1.000 33.02
ATOM	651	C	GLY			6150	2274	-1716 851 - 956
ANISOU				92	-15.223		66.572	1.000 26.22
		C	GLY	92	2603	5046	2314	-885 741 -947
ATOM	652	0	GLY	92	-16.289	13.666	65.939	1.000 23.91
ANISOU		0	GLY	92	2490	3396	3198	-680 548 -567
MOTA	653	N	SER	93	-14.010	13.956	66.088	1.000 23.77
ANISOU	653	N	SER	93	2405	3917	2708	-372 736 -560
ATOM	654	CA	SER	93	-13.801		64.690	1.000 23.41
ANISOU	654	CA	SER	93	2700	3292	2901	-386 970 -399
ATOM	655	C	SER	93	-12.410		64.240	
ANISOU		Č	SER	93	2547			1.000 24.26
ATOM	656	0				3908	2763	-286 833 -224
			SER	93	-11.497		65.089	1.000 27.06
ANISOU		0	SER	93	3401	3536	3346	630 92 - 386
ATOM	657	CB	SER	93	-13.966		64.467	1.000 25.71
ANISOU		CB	SER	93	2811	3225	3735	-576 271 -506
ATOM	658	OG	SER	93	-13.558	16.158	63.150	1.000 28.14
ANISOU	658	OG	SER	93	2694	3713	4284	-373 290 517
ATOM	659	N	TYR	94	-12.254		62.949	1.000 24.24
ANISOU	659	N	TYR	94	2786	3320	3104	-204 791 -817
ATOM	660	CA	TYR	94	-10.878		62.498	1.000 23.94
ANISOU		CA	TYR	94	3089	2502		
ATOM	661	C	TYR	94			3505	95 1112 - 683
ANISOU		C			-10.017		62.584	1.000 25.19
ATOM			TYR	94	2601	2657	4312	147 737 -625
	662	0	TYR	94	-8.786	14.421	62.694	1.000 30.11
ANISOU		0	TYR	94	2617	3095	5726	307 760 3 6
MOTA	663	CB	TYR	94	-10.800	12.659	61.098	1.000 25.64
ANISOU		CB	TYR	94	3566	2910	3267	-293 1331 - 525
ATOM	664	CG	TYR	94	-11.600		60.876	1.000 23.22
ANISOU	664	CG	TYR	94	3359	2768	2697	-69 784 -274
MOTA	665		TYR	94	-12.451		59.777	1.000 26.01
ANISOU			TYR	94	4410	2730		
ATOM	666		TYR	94	-11.564		2741	499 353 - 543
ANISOU			TYR				61.635	1.000 24.42
ATOM	667			94	3117	2866	3297	73 458 - 1 4
		CE1	TYR	94	-13.243		59.443	1.000 28.75
ANISOU		CE1	TYR	94	4559	3328	3037	434 140 -1370
ATOM	668	CE2	TYR	94	-12.375	9.159	61.305	1.000 26.47
ANISOU			TYR	94	4707	2585	2764	-220 1227 - 718
ATOM	669	CZ	TYR	94	-13.209		60.212	1.000 29.70
ANISOU	669	CZ	TYR	94	5641	3518	2125	-1172 1103 - 1447
ATOM	670	ОН	TYR	94	-14.059		59.730	1.000 34.02
ANISOU		ОН	TYR	94	3079	3962	5886	
ATOM	671	N	SER	95	-10.628		62.561	-423 1593 - 2638 1 000 22 61
ANISOU		N	SER	95	2460			1.000 22.61
			~ L. L.	ر ر	2400	2497	3632	-54 59 - 338

- 112 -16.975 62.750 1.000 22.54 -9.924 95 ATOM 672 CASER 2603 3706 -120 -301 4 6 95 2257 ANISOU 672 CASER 64.163 1.000 23.58 С 95 -9.370 17.106 673 SER ATOM -521 -88 -85 3478 3671 ANISOU 673 С SER 95 1811 18.034 64.481 1.000 26.53 95 -8.623 674 SER ATOM 0 -469 -167 -641 ANISOU 674 4247 0 SER 95 2592 3242 62.478 1.000 27.58 95 -10.838 18.177 675 CВ SER ATOM 365 -379 2 8 ANISOU 675 CB SER 95 3657 2556 4264 -11.506 18.093 61.242 1.000 39.40 676 OG 95 ATOM SER 900 -1445 1442 95 4214 4421 ANISOU 676 OG SER 6336 16.194 65.060 1.000 25.04 -9.712 677 N ASP 96 ATOM -399 277 -232 2579 3688 3248 ANISOU 677 NASP 96 -9.228 16.317 66.422 1.000 24.42 678 CA ASP 96 MOTA -470 257 -526 2603 3347 3330 ANISOU 678 CA ASP 96 96 -7.735 16.050 66.501 1.000 24.45 679 C ASP MOTA 96 -471 162 -383ANISOU 679 С ASP 2597 3228 3466 -7.073 16.589 67.404 1.000 26.51 ASP 96 680 O ATOM -170 160 -798 3370 ANISCU 680 0 ASP 96 2656 4047 -9.952 15.334 67.334 1.000 24.97 96 681 CB ASP ATOM -423 -228 7 7 ANISOU 681 CB ASP 96 2310 3806 3371 -11.411 15.605 67.606 1.000 26.77 CG ASP 96 ATOM 682 -362 -240 7 1 6 3566 ANISOU 682 CG ASP 96 2272 4334 -11.935 16.723 67.388 1.000 33.94 OD1 ASP 96 ATOM 683 204 569 4733 647 96 3267 4894 ANISOU 683 OD1 ASP -12.058 14.646 68.083 1.000 32.65 ATOM 684 OD2 ASP 96 4072 -1032 1446 - 202 3624 4709 ANISOU 684 96 OD2 ASP 15.226 65.581 1.000 22.21 97 -7.254 TYR 685 ATOM N -376 -77 -102 3389 2760 TYR 97 2292 ANISOU 685 N 14.852 65.583 1.000 23.71 97 -5.835 MOTA 686 CATYR 106 644 ANISOU 686 TYR 97 2480 3542 2987 -27 CA15.828 64.743 1.000 23.06 97 MOTA 687 C TYR -5.026 -410 -78 350 ANISOU 687 C 97 2363 3754 2647 TYR 16.327 65.230 1.000 24.29 MOTA 688 0 TYR 97 -3.992 97 3845 3178 -133 -230 7 4 2205 ANISOU 688 0 TYR -5.585 13.451 65.035 1.000 28.38 TYR 97 689 СВ ATOM 3324 4229 540 -450832ANISOU 689 CB TYR 97 3230 -4.132 13.025 65.082 1.000 30.37 690 TYR 97 CG MOTA -191 6 7 1 TYR 97 766 ANISOU 690 CG 3278 4101 4161 -3.511 12.691 66.285 1.000 30.19 CD1 TYR 97 MOTA 691 1106 151 951 ANISOU 691 CD1 TYR 97 2878 4475 4119 97 -3.370 12.945 63.922 1.000 29.79 ATOM 692 CD2 TYR 97 53 - 253 544 3997 4005 ANISOU 692 CD2 TYR 3317 97 -2.178 12.294 66.324 1.000 32.77 CE1 TYR ATOM 693 574 -68 763 ANISOU 693 CE1 TYR 97 2554 4771 5126 12.553 63.955 1.000 32.68 97 MOTA 694 CE2 TYR -2.043 5087 353 323 403 97 3793 ANISOU 694 CE2 TYR 3536 -1.445 12.228 65.157 1.000 33.00 MOTA 695 СZ TYR 97 1066 264 456 4284 5622 ANISOU 695 CZTYR 97 2633 -0.121 11.845 65.156 1.000 42.66 696 TYR 97 MOTA OH1161 764 1277 97 5373 8264 TYR 2572 ANISOU 696 ОН -3.465 16.575 62.134 1.000 23.20 MOTA 697 SER 98 CВ 2 - 5 4 4 ANISOU 697 SER 98 2461 2766 3587 105 CB -3.632 15.649 61.078 1.000 26.49 MOTA 698 OG SER 98 -154 238 -457 3059 3180 ANISOU 698 OG SER 98 3824 -5.694 17.744 61.701 1.000 18.66 MOTA 699 С SER 98 -295 66 1 3 С 2150 2637 ANISOU 699 SER 98 2301 -6.768 17.212 61.413 1.000 20.88 700 0 SER 98 ATOM -945 -249 1 8 1 2646 98 2245 ANISOU 700 0 SER 3042 16.110 63.511 1.000 23.62 98 -5.457 MOTA 701 N SER -441 -395 6 0 5 98 3227 2931 ANISOU 701 SER 2816 Ν -4.748 17.143 62.741 1.000 21.31 98 MOTA 702 CASER

- 113 -ANISOU 702 CA SER 98 2430 2687 133 2982 153 294 703 MET 99 -5.307 18.891 61.148 1.000 18.68 ANISOU 703 MET 99 2392 2722 1984 -978 -366 1 0 1 704 CAMET 99 -6.047 19.560 60.075 1.000 17.84 ANISOU 704 CAMET 99 2431 2620 1726 -945 -212 -17ATOM 705 CB MET 99 20.779 60.585 1.000 19.71 -6.819 ANISOU 705 СВ MET 99 2348 2968 2173 -679 25 6 4 ATOM 706 CG MET 99 20.392 61.374 1.000 23.68 -8.052 ANISOU 706 CG MET 99 2360 3055 3582 -504 393 489 ATOM 707 SD MET 99 -9.031 21.821 61.911 1.000 22.33 ANISOU 707 SD MET 99 2569 3383 2534 -522 170 -120 ATOM 708 CE MET 99 -8.148 22.225 63.419 1.000 36.98 ANISOU 708 CE ANISOU 708 CE ATOM 709 C ANISOU 709 C ATOM 710 O ANISOU 710 O ATOM 711 N 99 MET 6485 4165 3401 -225 -1904 - 23 99 19.954 58.973 1.000 17.19 MET -5.070 2269 MET 99 2488 1776 -960 -194 - 201 MET 99 -3.964 20.341 59.324 1.000 16.93 1932 99 MET 2583 1919 -367 -208 - 241 100 -5.486 CYS 19.864 57.715 1.000 20.00 N ANISOU 711 CYS 100 3178 2683 1739 -1753 -358 1 6 6 20.181 56.554 1.000 16.64 712 ATOM CA CYS 100 -4.645 CA ANISOU 712 CYS 100 2213 2294 1817 -924 -563 4 6 8 713 CB ATOMCYS 100 -4.291 18.893 55.813 1.000 17.74 ANISOU 713 CB CYS 100 2161 2174 560 -765 1 0 5 3 2407 714 SG CYS MOTA 100 -3.035 18.928 54.552 1.000 33.56 ANISOU 714 SG ATOM 715 C ANISOU 715 C CYS 100 5244 3511 3997 414 1509 6 0 1 CYS 100 -5.347 21.121 55.590 1.000 13.48 CYS 100 1879 1415 1829 -68 240 - 91 ATOM 716 O ANISOU 716 O ATOM 717 N CYS 100 -6.585 21.127 55.496 1.000 14.49 CYS 100 1880 1952 1673 -497 -57 1 4 TYR 101 -4.589 21.921 54.852 1.000 13.35 ANISOU 717 N Υ YR 101 1721 1677 1673 -254 -78 4 9 MOTA 718 CA TYR 101 -5.016 22.753 53.755 1.000 10.27 ANISOU 718 CA ATOM 719 CB TYR 101 926 1498 1477 -15 -141 -231 TYR 101 -5.102 24.265 54.124 1.000 13.60 ANISOU 719 101 1626 СВ TYR 1513 2027 -48 322 - 236 101 -5.498 25.025 52.863 1.000 17.31 ATOM 720 CG TYR ANISOU 720 101 2373 CG TYR 1509 2694 -158 -103 1 9 3 CD1 TYR ATOM 721 101 -6.815 25.068 52.519 1.000 16.38 ANISOU 721 CD1 TYR 101 2464 752 3006 190 -227 5 5 CE1 TYR 722 ATOM 101 -7.307 25.715 51.412 1.000 17.01 ANISOU 722 CE1 TYR 101 2755 714 2993 -86 -416 122 101 -4.616 25.679 52.012 1.000 19.51 ATOM 723 CD2 TYR CD2 TYR ANISOU 723 101 3032 1533 2847 -1143 -594 4 7 5 CE2 TYR ATOM 724 101 -5.065 26.321 50.872 1.000 20.96 ANISOU 724 101 2802 CE2 TYR 1949 238 3211 112 725 101 -6.414 26.334 50.568 1.000 22.78 ATOM CZ TYR ANISOU 725 CZTYR 101 3238 2291 3126 -1228 -919 6 2 4 OH TYR 101 -6.875 26.986 49.442 1.000 23.10 MOTA 726 ANISOU 726 OH TYR 101 3141 3112 2522 -14 -129 4 2 9 MOTA 727 C TYR 101 -4.041 22.518 52.596 1.000 11.25 ANISOU 727 C TYR 101 1223 1398 1654 -323 103 -252 MOTA 728 O TYR 101 -2.823 22.677 52.787 1.000 12.23 ANISOU 728 O TYR 101 1114 1750 1784 -87 130 - 20 ATOM 729 SER 102 -4.542 22.190 51.405 1.000 11.17 N ANISOU 729 N SER 102 1355 1279 1611 -220 145 - 263ATOM 730 CA SER 102 -3.752 21.802 50.235 1.000 10.46 ANISOU 730 CA SER 102 1144 1263 1568 62 -1 -125 ATOM 731 CB SER 102 -4.027 20.343 49.908 1.000 13.46 ANISOU 731 CB SER 102 1668 1212 2234 324 105 - 301 ATOM 732 OG SER 102 -3.723 19.487 51.025 1.000 16.42 ANISOU 732 OG SER 102 2291 1313 2637 -122 -43 9 6

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			SER	102	-4.046	22.668	49.008	1.000 11.74
			SER		1346	1500		18 - 39 - 10
			SER		-5.148	23.148		1.000 12.84
ANISOU 7			SER		1480	1410	1988	90 -66 2 4 9
			MET		-3.004	22.871		1.000 12.33
ANISOU 7			MET		1554	1722	1409	-262 -10 -246
ATOM 7 ANISOU 7			MET		-3.188	23.603		1.000 12.92
			MET		1663 -3.215	1681	1565	22 47 - 7 0
ANISOU 7			MET MET		2439	25.122 1634	47.179 2579	1.000 17.51
			MET		-1.929	25.808	47.549	-363 812 - 44 1.000 20.07
ANISOU 7			MET		2509	1470	3646	-538 688 376
			MET		-2.136	27.614	47.689	1.000 18.10
ANISOU 7			MET		2235	1665	2975	-3 -334 - 352
ATOM 7			MET		-2.365	28.068		1.000 18.09
ANISOU 7	40		MET		2319	1457	3098	-187 -718 - 214
ATOM 7			MET	103	-2.152	23.221		1.000 12.57
ANISOU 7			MET	103	1420	1837	1519	119 -53 238
			MET		-1.120	22.573	46.175	1.000 12.57
ANISOU 7			MET		1094	1891	1792	-155 -165 2 7 6
			GLY		-2.418	23.650		1.000 12.83
ANISOU 7			GLY		1493	1958	1422	237 -124 - 3 4
ATOM 7 ANISOU 7			GLY		-1.533	23.459	43.513	1.000 12.65
			GLY GLY		1075	2188	1544	-93 -37 242
ANISOU 7			GLY		-1.624 1909	24.622 1985	42.542 1561	1.000 14.36 -265 -294 1 4 2
			GLY		-2.033	25.700		1.000 15.69
ANISOU 7			GLY		1628	2273	2060	163 -197 2 1 3
ATOM 7			THR		-1.242	24.397	41.276	1.000 14.52
ANISOU 7	747		THR		1829	2182	1504	-59 -375 3 1 9
		CA	THR	105	-1.218	25.452	40.279	1.000 15.27
ANISOU 7			THR		1977	2223	1603	-105 -363 3 6 5
		СВ	THR		-0.359	25.083	39.039	1.000 15.61
ANISOU 7		CB	THR		1936	2122	1873	-37 -106 5 5 4
		OG1			-0.884	23.876		1.000 16.16
ANISOU 7		OG1			1738	2260	2140	217 -285 1 5 1
ANISOU 7		CG2 CG2			1.092	24.882	39.369	1.000 17.47
		CGZ	THR		1918 -2.603	2871 25.828	1847 39.755	-293 -227 5 2 7
ANISOU 7		C	THR		1989	1694	1913	1.000 14.73 122 -340 1 9 9
		Ō	THR		-2.730	26.921		1.000 19.91
ANISOU 7		0	THR		2579	2355	2632	23 -437 1004
ATOM 7	754	N						1.000 16.57
ANISOU 7			ALA					2 -260 661
		CA	ALA					1.000 14.94
ANISOU 7		CA	ALA		1975	1904	1798	105 -456 3 6 5
		CB	ALA		-5.054	24.945		1.000 17.75
ANISOU 7		CB	ALA		2006	2862		140 -201 - 3 2
ATOM 7	757	C	ALA		-5.942	24.251		1.000 16.26
	758	C	ALA		1710	2174	2293	327 -127 4 9 1
ANISOU 7		0	ALA ALA		-5.498 1622	23.398 1971	41.013 1945	1.000 14.57 213 -21 337
	759	N	ASP		-7.253			1.000 16.71
ANISOU 7		N	ASP		1768	2096		540 -22 3 0 4
	760	CA	ASP		-8.310	23.638		1.000 16.10
ANISOU 7	760	CA	ASP		1696	2175		51 -485 - 14
	761	CB	ASP		-8.231	22.171		1.000 17.09
ANISOU 7		CB	ASP	107	1299	2385	2808	144 -203 - 399
	762	CG	ASP		-8.418	21.966		1.000 21.54
ANISOU T		CG	ASP		2385	2894		84 - 317 - 722
ATOM 7	763	ODI	ASP	107	-9.452	22.445	38.189	1.000 23.92

ANISOU 763				145	
ANISOU 787 CD1 PHE 110 1885 2462 3387 461 573 - 70 7 87 7 7 88 7 8 7 8 8 7 8 7 9 1.000 20 .31 8 1 9 9 1 9 1 9 1 9 1 9 1 9 1 9 1 9 1	ATOM 764 ANISOU 764 ANISOU 765 ANISOU 765 ANISOU 766 ANISOU 767 ANISOU 767 ANISOU 768 ANISOU 768 ANISOU 769 ANISOU 770 ANISOU 770 ANISOU 771 ANISOU 771 ANISOU 771 ANISOU 772 ANISOU 772 ANISOU 773 ANISOU 773 ANISOU 773 ANISOU 773 ANISOU 774 ANISOU 775 ANISOU 775 ANISOU 776 ANISOU 777 ANISOU 778 ANISOU 778 ANISOU 778 ANISOU 779 ANISOU 779 ANISOU 779 ANISOU 780 ANISOU 781 ANISOU 782 ANISOU 783 ANISOU 783 ANISOU 784 ANISOU 784 ANISOU 785 ANISOU 786 ANISOU 787 ANISOU 7884 ANISOU 7885 ANISOU 7886 ANISOU 7886 ANISOU 7886 ANISOU 7886	ODZ ASP ODZ ASP C ASP O ASP O ASP O ASP O ASP O ASP O ASN N ASN CA ASN CA ASN CB CB ASN CB C	107 3447 107 -7.563 107 -8.285 107 1261 107 -8.507 107 2017 108 -8.027 108 2093 108 -7.967 108 1479 108 -6.925 108 1593 108 -5.516 108 1593 108 -5.516 108 1412 108 -4.823 108 -9.310 108 1471 108 -10.222 108 1861 109 -9.412 109 1458 109 -11.187 109 1458 109 -11.580 109 1593 109 -11.580 109 1593 109 -11.580 109 1593 109 -11.780 109 2460 109 -12.780 109 3055 109 -10.203 109 1179 109 2460 109 -9.416 100 -9.466 110 1369 110 -10.706 110 1369 110 -10.298 110 1626 110 -9.660 110 1423 110 -8.425 110 1702	21.311 38.08 4004 2954 23.785 42.16 1918 2201 22.850 42.93 1927 2390 25.020 42.59 1866 1870 25.314 44.03 1823 44.03 1823 44.03 1823 44.39 25.942 43.96 2141 24.50 224.49 44.64 25.708 44.64 2198 26.52 44.64 43.95 2219 45.95 1648 1994 25.796 46.76 2122 45.95 1648 1994 25.796 46.76 2122 1923 24.499 47.33 22.083 47.08 23.783 2403 24.499 47.38 25.794 47.86 23.783 45.52 24.48 47.08 27.99 48.73 26.42 47.16 27.99 47.16 30.25 47.16 30.27 47.16 30.27 47.16 30.27 47	1.000 24 . 8 8 105
ANISOU 784 CA PHE 110 1626 1801 3050 -116 259 -362 ATOM 785 CB PHE 110 -9.660 30.259 47.991 1.000 17.94 ANISOU 785 CB PHE 110 1423 2366 3027 -290 228 -129 ATOM 786 CG PHE 110 -8.425 29.972 47.165 1.000 20.32 ANISOU 786 CG PHE 110 1702 2650 3368 -176 459 -389 ATOM 787 CD1 PHE 110 -7.257 29.598 47.793 1.000 20.35 ANISOU 787 CD1 PHE 110 1885 2462 3387 461 573 -707 ATOM 788 CD2 PHE 110 -8.405 30.110 45.789 1.000 20.31 ANISOU 788 CD2 PHE 110 2073 2226 3419 512 712 -267 ATOM 789 CE1 PHE 110 -6.102 29.347 47.065 1.000 19.49 ANISOU 789 CE1 PHE 110 1958 2116 3332 176 749 -633 ATOM 790 CE2 PHE 110 -7.288 29.846 45.050 1.000 20.65 ANISOU 790 CE2 PHE 110 -7.288 29.846 45.050 1.000 20.65 ANISOU 791 CZ PHE 110 -6.118 29.496 45.694 1.000 19.43 ANISOU 791 CZ PHE 110 1925 2131 3327 219 542 -786 ATOM 792 C PHE 110 -11.495 29.556 49.538 1.000 17.08	ATOM 782 ANISOU 782 ATOM 783 ANISOU 783	O LEU O LEU N PHE N PHE	109 -9.416 109 2196 110 -10.706 110 1369	26.428 48.71 2210 1730 28.025 47.78 2042 2709	17 1.000 16.15 -52 -366 3 2 36 1.000 16.11 105 -118 - 288
ANISOU 787 CD1 PHE 110 1885 2462 3387 461 573 - 70 ATOM 788 CD2 PHE 110 -8.405 30.110 45.789 1.000 20.31 ANISOU 788 CD2 PHE 110 2073 2226 3419 512 712 - 26 ATOM 789 CE1 PHE 110 -6.102 29.347 47.065 1.000 19.49 ANISOU 789 CE1 PHE 110 1958 2116 3332 176 749 - 63 ATOM 790 CE2 PHE 110 -7.288 29.846 45.050 1.000 20.65 ANISOU 790 CE2 PHE 110 2158 2094 3596 758 724 - 32 ATOM 791 CZ PHE 110 -6.118 29.496 45.694 1.000 19.43 ANISOU 791 CZ PHE 110 1925 2131 3327 219 542 - 78 ATOM 792 C PHE 110 -11.495 29.556 49.538 1.000 17.08	ANISOU 784 ATOM 785 ANISOU 785 ATOM 786 ANISOU 786	CA PHE CB PHE CG PHE CG PHE	110 1626 110 -9.660 110 1423 110 -8.425 110 1702	1801 3050 30.259 47.99 2366 3027 29.972 47.16 2650 3368	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$
ATOM 793 O PHE 110 -12.562 29.792 48.929 1.000 21.26	ANISOU 787 ATOM 788 ANISOU 788 ATOM 789 ANISOU 789 ATOM 790 ANISOU 790 ATOM 791 ANISOU 791 ATOM 792 ANISOU 792 ANISOU 793	CD1 PHE CD2 PHE CD2 PHE CE1 PHE CE2 PHE CZ PHE CZ PHE CZ PHE CZ PHE C PHE C PHE C PHE	110 1885 110 -8.405 110 2073 110 -6.102 110 1958 110 -7.288 110 2158 110 -6.118 110 1925 110 -11.495 110 1774 110 -12.562	2462 3387 30.110 45.78 2226 3419 29.347 47.00 2116 3332 29.846 45.09 2094 3596 29.496 45.69 2131 3327 29.556 49.50 1806 2911 29.792 48.99	461 573 - 707 39 1.000 20.31 512 712 - 264 55 1.000 19.49 176 749 - 631 50 1.000 20.65 758 724 - 321 94 1.000 19.43 219 542 - 780 38 1.000 17.08 -74 414 - 111

- 116 -794 ATOM N PRO 111 -11.406 29.717 50.851 1.000 19.41 ANISOU 794 PRO 111 2279 N 2110 2985 -386 519 -314 795 CD PRO 111 -10.278 29.322 51.705 1.000 19.20 ANISOU 795 CD PRO 111 2773 1880 2640 -417 255 - 514 796 CA PRO 111 -12.549 30.252 51.604 1.000 21.47 ANISOU 796 CA PRO 111 3026 1924 3206 -50 728 ATOM 797 CB PRO 111 -12.167 30.007 53.055 1.000 23.63 ANISOU 797 CB PRO 111 3789 2054 3137 334 776 - 575 798 CG PRO 111 -10.775 29.535 53.100 1.000 22.33 ATOM ANISOU 798 CG PRO 111 2767 2908 2809 -1006 623 - 414 ATOM 799 C PRO 111 -12.828 31.739 51.433 1.000 23.88 ANISOU 799 C PRO 111 3139 2049 3887 79 -142 - 47 ATOM 800 O PRO 111 -13.919 32.194 51.834 1.000 26.77 ANISOU 800 O PRO 111 3800 2818 3555 992 -91 -3 ATOM 801 N SER 112 -11.906 32.517 50.872 1.000 25.19 ANISOU 801 N SER 112 3514 2269 3788 -247 -856 28 ATOM 802 CA SER 112 -12.300 33.919 50.631 1.000 26.43 ANISOU 802 CA SER 112 2654 2655 4734 496 1364 45 ATOM 803 CB SER 112 2654 2655 4734 496 1364 45 ATOM 803 CB SER 112 3122 3663 5895 172 2582 -5 ATOM 804 OG SER 112 3122 3663 5895 172 2582 -5 ATOM 804 OG SER 112 -11.322 34.719 52.688 1.000 36.94 ANISOU 804 OG SER 112 6530 2154 5351 1399 206 -4 ATOM 805 C SER 112 -11.262 34.587 49.723 1.000 26.62 ANISOU 805 C SER 112 2613 2546 4956 1021 1668 65 ATOM 806 O SER 112 -10.219 34.029 49.414 1.000 22.81 799 C PRO 111 -12.828 31.739 51.433 1.000 23.88 ATOM 3887 79 -142 - 479 -91 -397 -247 -856 2 8 2 1364 4 5 6 ANISOU 803 CB
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ANISOU 813 CB ASP 113 -8.294 36.790 48.459 1.000 25.85 113 2920 857 2317 4585 450 - 203114 -9.479 37.145 50.365 1.000 29.56

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 114 3189
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 114 -8.628
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 114 5580
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 114 -7.904
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 114 6798
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 1104 7 6 0 1028 1584 5 4 2 ASP ANISOU 813 CB 1774 1691 - 240 ASP ATOM 814 CG CG ASP OD1 ASP ANISOU 814 CG 693 - 248 MOTA 815 ANISOU 815 OD1 ASP 1703 931 - 913 ATOM 816 OD2 ASP 114 -6.932 39.178 53.622 1.000 54.35 114 5258 7609 7783 -868 495 1 114 -7.310 36.281 51.231 1.000 23.05 ANISOU 816 OD2 ASP -868 495 1602 ATOM 817 C ASP ANISOU 817 C 114 2621 ASP 2102 4033 444 1874 3 4 0 ASP 114 -6.111 36.371 50.955 1.000 22.05 818 0 ATOM ASP 114 2423 ANISOU 818 O 2277 3677 131 1411 - 461 ATOM 819 N PHE 115 -7.854 35.160 51.637 1.000 23.21 ANISOU 819 N PHE 115 2945 1890 3984 -130 1293 - 228 ATOM 820 CA PHE 115 -7.120 33.896 51.690 1.000 19.93 ANISOU 820 CA PHE 115 2562 1908 3102 -198 655 -294 ATOM 821 115 -8.085 32.792 52.157 1.000 19.49 CB PHE ANISOU 821 CB PHE 115 2378 1754 3275 64 881 - 314 ATOM 822 CG PHE 115 -7.523 31.445 52.540 1.000 17.25 ANISOU 822 CG PHE 115 2053 1589 2912 -56 348 - 695 ATOM 823 CD1 PHE 115 -7.637 30.951 53.833 1.000 19.00 ANISOU 823 CD1 PHE 115 2728 1539 2950 73 496 -683 ATOM 824 CD2 PHE 115 -6.868 30.634 51.615 1.000 17.88

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CD2 PHE 115 1933 ANISOU 824 1931 2927 7 298 -810 29.711 54.163 1.000 20.25 825 CE1 PHE 115 -7.100 ANISOU 825 3042 CE1 PHE 115 2825 1825 317 341 - 575826 CE2 PHE 115 -6.338 29.412 51.955 1.000 19.11 MOTA CE2 PHE ANISCU 826 115 1865 2158 3237 336 351 -885 827 CZ PHE 115 -6.452 MOTA 28.936 53.233 1.000 19.39 ANISOU 827 CZ PHE 115 2068 1910 3390 320 248 - 669 115 -6.506 33.624 50.327 1.000 17.86 828 C ATOM PHE ANISOU 828 C ATOM 829 O PHE 115 1964 1945 2878 61 344 1 6 115 -5.324 33.315 50.271 1.000 17.34 PHE ANISOU 829 O PHE 115 1868 2107 -132 179 157 2613 830 N GLU 116 -7.310 33.683 49.263 1.000 18.21 ATOM ANISOU 830 N GLU 116 1921 1934 3065 547 281 6 2 MOTA 831 CA GLU 116 -6.848 33.387 47.907 1.000 19.99 ANISOU 831 CA GLU 116 2128 2618 2851 81 231 2 2 2 116 -7.968 33.605 46.884 1.000 18.61 MOTA 832 CB GLU ANISOU 832 CB GLU 116 2058 1952 3060 231 GLU 116 -7.398 33.378 45.482 1.000 18.61 833 CG MOTA ANISOU 833 CG GLU 116 1813 2288 2971 295 834 CD GLU 116 -8.442 33.230 44.412 1.000 22.40 ATOM 116 1908 3193 3410 -122 -278 -116 -9.654 33.272 44.678 1.000 30.82 ANISOU 834 CD GLU -122 -278 - 91835 OE1 GLU ATOM GLU 116 -9.654 33.272 44.678 1.000 30.82 GLU 116 1793 4465 5452 273 -414 - 2 4 GLU 116 -8.085 33.063 43.225 1.000 30.24 GLU 116 3333 5132 3026 382 -658 3 2 7 GLU 116 -5.620 34.211 47.535 1.000 18.82 GLU 116 2090 2069 2990 294 119 4 8 7 GLU 116 -4.605 33.701 47.049 1.000 17.41 GLU 116 2228 1780 2606 45 259 2 8 2 ANISOU 835 OE1 GLU ATOM 836 OE2 GLU ANISOU 836 OE2 GLU С ATOM 837 ATOM 837 C
ANISOU 837 C
ATOM 838 O
ANISOU 838 O
ATOM 839 N
ANISOU 839 N ARG 117 2313 ARG 2185 3487 408 220 9 0 117 2313 2185 3487 408 220 9 117 -4.560 36.420 47.431 1.000 21.35 ATOM 840 CA ARG ANISOU 840 CA ARG ATOM 117 2337 1800 3976 466 147 - 31 117 -3.291 36.054 48.192 1.000 20.52 841 C MOTA ARG 117 2292 2124 ANISOU 841 C ARG 3380 353 288 - 10 842 0 117 -2.186 35.969 47.636 1.000 18.96 ATOM ARG 117 2223 1664 ANISOU 842 O ARG 3316 138 318 231 843 CB ARG 117 -4.971 37.885 47.693 1.000 25.59 ATOM ANISOU 843 CB ARG 117 3237 1900 4587 929 1882 6 3 2 844 CG ARG 117 -3.881 38.908 47.478 1.000 32.57 MOTA ANISOU 844 CG ARG 117 5212 1925 5237 -281 1083 6 2 3 ATOM 845 CD ARG 117 -4.325 40.323 47.859 1.000 36.56 ANISOU 845 CD ARG 117 6009 2157 5724 149 1774 6 ATOM 846 NE ARG 117 -5.162 40.335 49.056 1.000 44.43 1774 6 6 3 ANISOU 846 NE ARG 117 7200 3742 5940 -96 2344 -ATOM 847 CZ ARG 117 -4.763 40.501 50.306 1.000 45.48 ANISOU 847 CZ ARG 117 6422 4804 6054 -370 2388 -2344 - 15117 6422 4804 6054 -370 2388 -1 117 -3.484 40.683 50.619 1.000 53.21 117 6867 6451 6900 -2543 2487 3 117 -5.647 40.487 51.301 1.000 50.00 117 6265 6511 6220 224 2433 --370 2388 - 283MOTA 848 NH1 ARG -2543 2487 3 5 4 ANISOU 848 NH1 ARG ATOM 849 NH2 ARG ANISOU 849 NH2 ARG 2433 - 1534 118 -3.439 35.832 49.493 1.000 19.30 118 2275 1838 3221 128 407 -645 850 N MOTA ILE ANISOU 850 N ILE CA ILE 118 -2.275 35.527 50.331 1.000 18.25 MOTA 851 ANISOU 851 CA ILE 118 2376 78 530 - 449 1745 2811 MOTA 852 CB ILE 118 -2.665 35.597 51.820 1.000 18.24 ANISOU 852 CB ILE 118 2201 1726 3003 906 - 306 346 118 -1.712 34.851 52.732 1.000 18.49 853 CG2 ILE CG2 ILE ANISOU 853 118 2077 2158 2792 -202 308 -530 118 -2.877 37.031 52.368 1.000 24.69 MOTA 854 CG1 ILE ANISOU 854 CG1 ILE 118 4436 1808 3136 284 1382 - 414

- 118 -855 CD1 ILE 118 -3.786 37.025 53.582 1.000 29.63 ATOM ANISOU 855 CD1 ILE 118 6169 3096 1994 1258 - 1068 189 ILE 118 -1.692 MOTA 856 C 34.172 49.959 1.000 15.65 ANISOU 856 C ILE 118 2316 1549 2082 -89 573 - 117 118 -0.463 34.035 49.802 1.000 14.59 ATOM 857 O ILE ANISOU 857 O ILE 118 2240 1255 2051 16 286 214 858 N TRP 119 -2.523 33.139 49.784 1.000 14.44 ATOM ANISOU 858 N TRP 119 2125 1592 1771 47 128 - 7 1 859 CA TRP 119 -2.010 31.795 49.518 1.000 13.68 ATOM ANISOU 859 CA TRP 119 1712 1529 1957 -61 220 4 0 860 CB TRP 119 -3.089 30.755 49.932 1.000 14.93 ATOM ANISOU 860 CB TRP 119 1819 1729 2123 -234 295 - 35 ATOM 861 CG TRP 119 -2.864 30.482 51.420 1.000 16.19 ANISOU 861 CG TRP 119 1640 2364 2146 -168 582 1 ATOM 862 CD2 TRP 119 -2.116 29.430 51.993 1.000 20.41 ANISOU 862 CD2 TRP 119 3189 2414 2151 202 523 4 2364 2146 -168 582 167 523 405 CD2 TRP 119 3189 2414 2151 202 523 4 0 5 CE2 TRP 119 -2.177 29.580 53.392 1.000 19.84 CE2 TRP 119 3536 1818 2184 -439 234 1 3 7 CE3 TRP 119 -1.390 28.357 51.456 1.000 23.94 CE3 TRP 119 5382 1647 2068 561 126 4 0 0 CD1 TRP 119 -3.340 31.223 52.460 1.000 20.05 CD1 TRP 119 3207 2343 2069 -9 189 -1 3 9 NE1 TRP 119 -2.938 30.689 53.649 1.000 20.32 NE1 TRP 119 2806 2726 2188 -96 -68 -18 ATOM 863 ANISOU 863 ATOM 864 ANISOU 864 ATOM 865 ANISOU 865 ATOM 866 119 2806 2726 2188 -96 -68 -185 119 -1.547 28.714 54.281 1.000 22.12 NE1 TRP ANISOU 866 CZ2 TRP ATOM 867 CZ2 TRP 119 4071 2256 2078 -17 105 2 2 119 -0.761 27.490 52.332 1.000 21.52 ANISOU 867 ATOMCZ3 TRP 868 ANISOU 868 CZ3 TRP 119 4214 2168 1794 311 -193 1 ATOM 869 CH2 TRP 119 -0.847 27.674 53.715 1.000 24.34 ANISOU 869 CH2 TRP 119 5349 2047 1850 329 148 1 ATOM 870 C TRP 119 -1.521 31.634 48.095 1.000 14.27 ANISOU 870 C TRP 119 2180 1259 1985 -187 334 -311 -193 1 9 7 329 148 183 U 870 C TRP 119 2180 1259 1985 -187 334 - 65 871 O TRP 119 -0.569 30.865 47.855 1.000 14.73 ATOM ANISOU 871 O TRP 119 1996 1653 1946 -67 362 1 ATOM 872 N THR 120 -2.109 32.325 47.116 1.000 13.99 ANISOU 872 N THR 120 2231 1237 1848 106 627 --67 362 101 ATOM 872 N THR 120 -2.109 32.325 47.116 1.000 13.99 ANISOU 872 N THR 120 2231 1237 1848 106 627 -1 ATOM 873 CA THR 120 -1.541 32.275 45.762 1.000 15.19 ANISOU 873 CA THR 120 1903 2093 1774 9 435 -242 ATOM 874 CB THR 120 1934 2304 1995 -331 152 6 ATOM 875 OG1 THR 120 1934 2304 1995 -331 152 6 ATOM 875 OG1 THR 120 1891 2288 2863 -236 195 48 ATOM 876 CG2 THR 120 1891 2288 2863 -236 195 48 ATOM 876 CG2 THR 120 -1.974 32.906 43.358 1.000 18.02 ANISOU 876 CG2 THR 120 -1.974 32.906 43.358 1.000 18.02 ANISOU 877 C THR 120 1868 2050 1475 87 285 -167 ATOM 878 O THR 120 1868 2050 1475 87 285 -167 ATOM 878 O THR 120 1864 1692 1620 301 354 2: ATOM 879 N GLN 121 0.114 33.962 46.429 1.000 14.55 ANISOU 879 N GLN 121 0.114 33.962 46.429 1.000 14.55 ANISOU 879 N GLN 121 1721 1672 2136 304 175 - ATOM 880 CA GLN 121 1.459 34.548 46.483 1.000 15.80 ANISOU 880 CA GLN 121 2.465 33.642 47.176 1.000 13.73 106 627 - 137 -331 152 6 6 -236 195 407 322 318 301 354 217 175 - 67 -119 3 6 2 GLN 121 2.465 33.642 47.176 1.000 13.73 ATOM 881 C ANISOU 881 C GLN 121 1747 1665 1806 -30 18 1 1 4 GLN 121 3.603 33.452 46.685 1.000 15.36 ATOM 882 Q ANISOU 882 O GLN 121 2063 1688 48 360 - 4 4 2084 883 CB GLN 121 1.315 35.918 47.154 1.000 18.85 MOTA ANISOU 883 CB GLN 121 2537 1426 3200 -73 -5 3 5 6 GLN 121 2.639 36.558 47.543 1.000 18.88 ATOM 884 CG ANISOU 884 CG GLN121 2507 1788 2878 59 9 - 248 ATOM 885 CD121 3.468 36.936 46.337 1.000 20.70 GLN

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		- 119 -	
ANISOU 885	CD GLN 121 2584	2138 3142	-373 -85 231
ATOM 886	OE1 GLN 121 2.935		
ANISOU 886	OE1 GLN 121 2.933		1.000 22.47
ATOM 887		2822 3019	-245 0 121
	NE2 GLN 121 4.779	37.101 46.522	1.000 25.22
ANISOU 887	NE2 GLN 121 2426	3344 3811	127 -131 1 3 8 5
ATOM 888	N TYR 122 2.081	33.054 48.299	1.000 12.26
ANISOU 888	N TYR 122 1747	1514 1399	99 - 55 - 258
ATOM 889	CA TYR 122 2.896	32.102 49.050	1.000 13.18
ANISOU 889	CA TYR 122 1901	1643 1464	-20 -253 - 160
ATOM 890	CB TYR 122 2.211	31.724 50.364	1.000 13.78
ANISOU 890	CB TYR 122 2045	1435 1756	116 48 - 28
ATOM 891	CG TYR 122 2.994	30.808 51.282	1.000 14.22
ANISOU 891	CG TYR 122 1966	1681 1758	101 68 1 0 1
ATOM 892	CD1 TYR 122 4.271	31.120 51.722	1.000 17.48
ANISOU 892	CD1 TYR 122 1788	1972 2882	
ATOM 893	CE1 TYR 122 5.003		149 -5 4 2 0
ANISOU 893	CE1 TYR 122 2131		1.000 18.55
		2050 2868	102 -404 2 5 1
ATOM 894		29.619 51.731	1.000 20.72
ANISOU 894	CD2 TYR 122 3308	1366 3197	-519 -1524 3 2 3
ATOM 895	CE2 TYR 122 3.140	28.773 52.574	1.000 25.40
ANISOU 895	CE2 TYR 122 3772	1812 4067	-782 -2084 873
ATOM 896	CZ TYR 122 4.413	29.101 52.992	1.000 20.93
ANISOU 896	CZ TYR 122 2985	1742 3224	- 96 <i>-</i> 1145 3 1 3
ATOM 897	OH TYR 122 5.068	28.230 53.826	1.000 29.87
ANISOU 897	OH TYR 122 4830	1998 4522	-680 -3078 621
ATOM 898	C TYR 122 3.218	30.876 48.209	1.000 12.33
ANISOU 898	C TYR 122 1833	1412 1439	89 -218 8 8
ATOM 899	O TYR 122 4.395	30.507 48.117	1.000 14.25
ANISOU 899	O TYR 122 1896	1861 1656	339 -242 2 1 6
ATOM 900	N PHE 123 2.224	30.269 47.573	1.000 11.28
ANISOU 900	N PHE 123 1950		
ATOM 901	CA PHE 123 2.482		6 -151 185
ANISOU 901		29.151 46.665	1.000 12.08
ATOM 902		1219 1640	01 00 2 0
ANISOU 902	CB PHE 123 1.139	28.719 46.024	1.000 13.86
	CB PHE 123 2048	1550 1666	-104 -276 - 82
ATOM 903	CG PHE 123 1.311	27.516 45.099	1.000 14.44
ANISOU 903	CG PHE 123 2173	1677 1637	142 -475 - 9 4
ATOM 904	CD1 PHE 123 1.281	26.234 45.614	1.000 13.64
ANISOU 904	CD1 PHE 123 1857	1563 1764	-42 -702 - 236
ATOM 905	CD2 PHE 123 1.511	27.664 43.729	1.000 13.81
ANISOU 905	CD2 PHE 123 1450	2164 1634	-420 -295 -248
ATOM 906	CE1 PHE 123 1.468	25.141 44.795	1.000 17.16
ANISOU 906	CE1 PHE 123 2282	1819 2418	130 -855 - 644
ATOM 907	CE2 PHE 123 1.715	26.559 42.916	1.000 18.31
ANISOU 907	CE2 PHE 123 2098	2657 2201	-1053 172 -845
ATOM 908	CZ PHE 123 1.706	25.295 43.445	1.000 16.71
ANISOU 908	CZ PHE 123 1442		
ATOM 909	C PHE 123 3.489		
ANISOU 909		29.511 45.581	1.000 13.48
		1472 1645	236 157 1 8
	O PHE 123 4.424	28.768 45.242	1.000 13.07
ANISOU 910	O PHE 123 1591	1498 1876	42 - 78 - 172
ATOM 911	N ASP 124 3.294	30.684 44.948	1.000 13.83
ANISOU 911	N ASP 124 1490	1575 2189	51 207 2 8 8
ATOM 912	CA ASP 124 4.207	31.036 43.861	1.000 13.75
ANISOU 912	CA ASP 124 1505	1330 2389	458 398 344
ATOM 913	CB ASP 124 3.708	32.352 43.242	1.000 18.95
ANISOU 913	CB ASP 124 2650	1970 2580	656 -63 926
ATOM 914	CG ASP 124 4.470	32.708 41.989	1.000 27.54
ANISOU 914	CG ASP 124 5327	2099 3036	-123 939 880
ATOM 915	OD1 ASP 124 3.541		
ANISOU 915			1.000 37.04
*747000 717	OD1 ASP 124 6362	3225 4485	108 2616 - 331

			- 120 -		
ATOM 916	OD2 ASP	124 4.985		42.011	1.000 32.60
ANISOU 916	OD2 ASP	124 4724		4151	-1539 234 8 5 1
ATOM 917	C ASP	124 5.645	31.164	44.328	1.000 14.49
ANISOU 917	C ASP	124 1493		2293	327 485 482
ATOM 918 ANISOU 918	O ASP O ASP	124 6.591 124 1477		43.674	
ATOM 919	N ARG	125 5.866		2679 45.499	289
ANISOU 919	N ARG	125 1501		2558	353 398 414
ATOM 920	CA ARG	125 7.214	31.863	46.044	
ANISOU 920	CA ARG	125 1642		2963	194 178 226
ATOM 921 ANISOU 921	C ARG C ARG	125 7.828 125 1396		46.346	
ATOM 922	O ARG	125 8.999		2496 46.034	232 -25 153 1.000 14.10
ANISOU 922	O ARG	125 1279		2424	7 -205 -201
ATOM 923	CB ARG	125 7.213	32.705	47.318	1.000 18.13
ANISOU 923 ATOM 924	CB ARG CG ARG	125 1950 125 7.045		3035	787 -81 4 6
ANISOU 924	CG ARG	125 7.045		47.041 4919	1.000 23.51 883 -36 -225
ATOM 925	CD ARG	125 8.391		46.694	
ANISOU 925	CD ARG	125 3596	2824	4724	-667 237 -187
ATOM 926	NE ARG	125 8.194	36.262	46.803	1.000 32.99
ANISOU 926 ATOM 927	NE ARG CZ ARG	125 4350 125 8.868		5418 47.495	-678 -1642 1 5 6
ANISOU 927	CZ ARG	125 2292		5353	1.000 27.38 -276 -580 - 246
ATOM 928	NH1 ARG	125 9.916			1.000 38.55
ANISOU 928	NH1 ARG	125 4611		6433	449 -2476 -669
ATOM 929 ANISOU 929	NH2 ARG NH2 ARG	125 8.491 125 4062		47.442	
ATOM 930	N GLN	126 7.065		4865 46.920	-369 -835 3 6 3 1.000 12.36
ANISOU 930	N GLN	126 1316	1376	2002	248 -63 -264
ATOM 931	CA GLN	126 7.524			1.000 13.39
ANISOU 931 ATOM 932	CA GLN CB AGLN	126 1765 126 6.363		1999	219 -355 - 377
ANISOU 932		126 2422		47.828 2357	0.500 16.24 188 202 -192
ATOM 933	CG AGLN	126 6.149	27.758	49.284	
ANISOU 933		126 2761	2021	2371	68 233 - 210
ATOM 934 ANISOU 934		126 7.077 126 3578	27.146 2745	50.298	
ATOM 935		126 7.181		2774 51.419	-604 -757 3 3 0.500 35.94
ANISOU 935	OE1 AGLN	126 6788		3136	-578 -1567 - 478
ATOM 936		126 7.774	26.055	50.008	0.500 24.63
ANISOU 936 ATOM 937		126 4491			-881 -2407 462
ANISOU 937		126 6.525 126 1695	27.417 1137	2245	0.500 13.36 602 -114 - 255
ATOM 938		126 6.604	27.750	49.497	
ANISOU 938		126 2537	2257	2153	-68 -176 - 105
ATOM 939 ANISOU 939		126 5.442	27.237	50.319	
ATOM 940		126 2227 126 5.605	2573 26.442	2198 51.242	344 -159 1 0 6 0.500 25.36
ANISOU 940		126 3289	3517	2828	-100 -223 9 5 3
ATOM 941		126 4.231	27.685	50.003	0.500 25.02
ANISOU 941 ATOM 942		126 2427	2669	4413	1004 -83 -298
ANISOU 942	C GLN C GLN	126 7.860 126 1506	27.448 1434	45.861 1979	1.000 12.95 307 -372 - 366
ATOM 943	O GLN	126 8.859	26.721	45.748	
ANISOU 943	O GLN	126 1461	1142	1827	182 -85 159
ATOM 944 ANISOU 944	N TYR N TYR	127 6.960	27.578	44.868	1.000 11.61
ATOM 945	N TYR CA TYR	127 1400 127 7.152	1276 26.869	1735 43.585	146 -168 - 10 1.000 11.21
ANISOU 945	CA TYR	127 1469	1242	1550	-92 -40 1 9 2
ATOM 946	CB TYR	127 5.901			1.000 11.82

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- 121 -
ANISOU 946
                   127 1346
           CB
              TYR
                               1655
                                                   82 4 7
                                      1491
                                              -13
      947
           CG
              TYR
                    127 5.791
                               26.069
                                      41.496 1.000 11.49
ANISOU 947
           CG
              TYR
                    127 1278
                               1428
                                      1660
                                              -4 -4 1 0
      948
           CD1 TYR
                    127 6.550
                               24.928 41.270 1.000 11.28
ANISOU 948
                    127 1030
           CD1 TYR
                               1334
                                      1921
                                             -87 -100 3 3
      949
                    127 6.406
ATOM
           CE1 TYR
                               24.153 40.115 1.000 11.47
ANISOU 949
           CE1 TYR
                    127 1164
                                             -51 -53 2 1
                               1167
                                      2027
      950
           CD2 TYR
                               26.410 40.500 1.000 11.98
ATOM
                    127 4.871
ANISOU 950
           CD2 TYR
                    127 1677
                               1093
                                             204 -219 -100
                                      1784
ATOM
      951
           CE2 TYR
                    127 4.715
                                      39.357 1.000 11.37
                               25.655
ANISOU 951
           CE2 TYR
                    127 1539
                               1118
                                      1665
                                              140 -68 - 73
ATOM
      952
           CZ
               TYR
                    127 5.494
                               24.508
                                      39.163 1.000 11.02
ANISOU 952
                    127 1202
           CZ
               TYR
                               1226
                                      1760
                                              91 48 - 125
      953
           ОН
ATOM
               TYR
                    127 5.379
                               23.720 38.030 1.000 11.57
          ОН
               TYR
ANISOU 953
                    127 1547
                               1138
                                      1712
                                              94 177 - 3 4
          C
MOTA
       954
               TYR
                    127 8.386
                               27.392 42.882 1.000 10.83
          С
ANISOU 954
               TYR
                    127 1296
                               989 1830
                                         230 -43 3 7 8
MOTA
       955
           0
               TYR
                    127 9.185
                               26.605 42.375 1.000 10.86
          0
ANISOU 955
               TYR
                    127 1292
                                            164 -237 - 42
                               1232
                                      1603
          N
MOTA
      956
               THR
                    128 8.565
                               28.716 42.865 1.000 10.98
ANISOU 956
          N
               THR
                    128 1554
                               976 1642
                                           212 -9 5 5 7
      957
               THR
                    128 9.766
                               29.305 42.295 1.000 11.80
ATOM
           CA
ANISOU 957
              THR
          CA
                   128 1686
                               1125
                                      1673
                                             -47 -169 3 8 6
                   128 9.605
ATOM
      958
          CB
               THR
                               30.849 42.378 1.000 12.66
ANISOU 958
          CB
               \mathtt{THR}
                   128 1873
                               1074
                                      1864
                                             -52 -233 5 2 1
ATOM
       959
           OG1 THR
                   128 8.530
                               31.286 41.517 1.000 16.74
ANISOU 959
           OG1 THR
                    128 2223
                               1597
                                      2542
                                              124 -457 9 9 8
ATOM
      960
          CG2 THR
                   128 10.878 31.510 41.893 1.000 16.54
ANISOU 960 CG2 THR
                    128 1871
                               778 3635
                                         262 655 1 3 8
ATOM
                   128 11.040 28.828 42.964 1.000 11.26
       961 C
               THR
ANISOU 961 C
               THR
                   128 1562
                               980 1738 -71 -162 148
ATOM
      962 O
               THR
                   128 11.995 28.458 42.258 1.000 12.16
ANISOU 962 O
               THR 128 1769
                               1092
                                      1758
                                             17 26 2 7 9
ATOM
       963
          N
               ALA 129 11.083 28.802 44.300 1.000 10.39
          N
ANISOU 963
               ALA 129 1183
                                      1763
                               1001
                                             70 -118 147
MOTA
       964
          CA ALA 129 12.273 28.386 45.037 1.000 10.59
ANISOU 964
           CA
               ALA 129 1206
                               945 1873 -69 -170 281
ATOM
       965
           CB
               ALA 129 12.113 28.603 46.536 1.000 12.46
ANISOU 965
           CB
                   129 2113
               ALA
                               851 1769 82 -218 577
          С
MOTA
       966
               ALA
                    129 12.575 26.906 44.802 1.000 11.35
ANISOU 966
           С
                               883 2170 -16 -141 410
               ALA
                    129 1258
ATOM
       967
           0
               ALA
                    129 13.738
                              26.485 44.641 1.000 10.93
                                      1796
ANISOU 967
          0
               ALA
                    129 1202
                                            -36 -213 1 2 1
                               1157
       968 N
MOTA
               SER
                    130 11.519
                               26.086 44.750 1.000 12.27
ANISOU 968
          N
                    130 1280
                               984 2398
               SER
                                          -65 \quad -1 \quad -24
           CA
ATOM
       969
                   130 11.682
               SER
                               24.650 44.512 1.000 10.89
ANISOU 969
          CA
               SER 130 1623
                               876 1638
                                          -85
                                                44 3 7 0
               ASER 130 10.342
MOTA
       970
           СВ
                               23.940 44.716 0.500 10.08
ANISOU 970
               ASER 130 1432
                               603 1793
           CB
                                           213
                                                 247 4 1 3
ATOM
       971
           OG
               ASER 130 9.771
                               24.063 46.006 0.500 9.12
ANISOU 971
           OG
               ASER 130 1021
                               651 1792 91 1 -143
       972
MOTA
           CB
               BSER 130 10.364
                               23.919 44.765 0.500 10.60
ANISOU 972
           CB
               BSER 130 1687
                               822 1521 -45 318 1 5 8
MOTA
       973
           OG
               BSER 130 9.418
                               24.098 43.734 0.500 16.22
ANISOU 973
           OG
               BSER 130 1717
                               1289
                                      3156
                                              137
       974
ATOM
           C
               SER 130 12.214
                               24.373 43.110 1.000 10.53
ANISOU 974
           С
               SER
                   130 1586
                               733 1684 -166 210 484
ATOM
       975
           0
               SER 130 13.137
                               23.532 42.942 1.000 11.17
ANISOU 975
           0
               SER 130 1385
                                      1849 -151 -95 140
                               1012
ATOM
       976
           Ν
               ARG
                    131 11.680
                               25.044 42.079 1.000 10.46
ANISOU 976
           N
               ARG
                    131 1578
                               861 1534 -87
                                                -66 9 9
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			120 "		
ANISOU 1007 C	G ARG	135 4204	1120	1980	-490 -433 1 5 0
ATOM 1008 C		135 17.237	26.563		1.000 22.14
ANISOU 1008 C					
		135 4046	1500	2868	-159 315 822
ATOM 1009 N		135 15.831	26.607	36.077	1.000 22.66
ANISOU 1009 N	E ARG	135 4239	1404	2965	-94 47 2 5 7
ATOM 1010 C		135 14.802	27.184		
				36.684	1.000 21.69
ANISOU 1010 C	_	135 4004	1906	2333	92 - 506 6 4
ATOM 1011 N		135 14.917	27.843	37.833	1.000 22.26
ANISOU 1011 N	H1 ARG	135 4114	2532	1812	460 -833 3 4 1
ATOM 1012 N		135 13.582	27.113	36.149	1.000 22.31
ANISOU 1012 N					
			2243	2234	-544 -419 8
ATOM 1013 C		135 19.251	23.275	39.057	1.000 12.70
ANISOU 1013 C	ARG	135 1742	1264	1821	-119 -16 430
ATOM 1014 O	ARG	135 20.069	22.818	38.238	1.000 14.67
ANISOU 1014 O		135 2133	1529		
ATOM 1015 N				1910	19 169 3 9 1
_		136 19.572	23.712	40.266	1.000 12.15
ANISOU 1015 N		136 1423	1372	1820	-36 70 4 3 0
ATOM 1016 C.	A GLU	136 20.960	23.630	40.763	1.000 14.52
ANISOU 1016 C		136 1622	1701	2194	-90 -197 3 7 1
ATOM 1017 C		136 21.212			
			24.513	41.981	1.000 15.59
ANISOU 1017 C		136 1502	1781	2642	14 -231 1 1
ATOM 1018 C	G GLU	136 21.064	26.020	41.783	1.000 18.01
ANISOU 1018 C	G GLU	136 2010	1762	3071	-232 -153 1 2 6
ATOM 1019 C		136 21.798	26.484	40.537	
ANISOU 1019 C		136 2071			1.000 20.18
			2079	3519	-308 89 3 6 9
		136 22.987	26.148	40.394	1.000 24.64
ANISOU 1020 O		136 2060	2937	4364	-262 338 615
ATOM 1021 O	E2 GLU	136 21.195	27.150	39.670	1.000 24.19
ANISOU 1021 O		136 2479	2327	4005	
ATOM 1022 C					-381 317 1426
		136 21.364	22.186	41.076	1.000 14.00
ANISOU 1022 C		136 1338	1619	2361	-112 -442 2 2 3
ATOM 1023 O	GLU	136 22.508	21.781	40.833	1.000 13.86
ANISOU 1023 O		136 1366	1890	2009	-100 -287 3 2 9
ATOM 1024 N		137 20.472			
·			21.338	41.580	1.000 11.78
ANISOU 1024 N		137 1309	1451	1715	148 -223 8 5
ATOM 1025 C		137 20.753	19.896	41.771	1.000 12.49
ANISOU 1025 C	A VAL	137 1369	1522	1853	240 -69 289
ATOM 1026 C		137 19.560	19.165	42.429	1.000 12.41
ANISOU 1026 C		137 1422	1424		
ATOM 1027 C				1869	-67 -85 -204
ATOM 1027 C		137 19.728	17.634	42.401	1.000 12.55
ANISOU 1027 C		137 1371	1508	1892	182 185 111
ATOM 1028 C	G2 VAL	137 19.355	19.607	43.852	1.000 11.35
ANISOU 1028 C	G2 VAL	137 1461	1281	1572	182 -254 2 8 8
ATOM 1029 C		137 21.100	19.241		1.000 12.48
ANISOU 1029 C					
		137 1202	1428	2113	150 -16 8 5
ATOM 1030 O		137 22.057	18.462		1.000 13.03
ANISOU 1030 O	VAL	137 1021	1683	2249	149 1 146
ATOM 1031 N	LEU	138 20.309	19.562	39.401	1.000 10.28
ANISOU 1031 N	LEU	138 1198	881 18		
ATOM 1032 C					
		138 20.571	19.029	38.066	1.000 12.48
ANISOU 1032 C		138 1312	1408	2024	110 273 - 52
ATOM 1033 C		138 19.398	19.358	37.130	1.000 11.81
ANISOU 1033 C	B LEU	138 1260	1586	1642	-20 383 4 3
ATOM 1034 C		138 18.036	18.726	37.457	
ANISOU 1034 C					1.000 10.77
		138 1391	1397	1304	-83 219 213
	D1 LEU	138 16.916	19.324	36.596	1.000 12.72
ANISOU 1035 C	Dl LEU	138 1416	1587	1829	-59 -25 173
ATOM 1036 C	D2 LEU	138 18.052	17.207	37.320	1.000 14.32
ANISOU 1036 C	D2 LEU	138 1986	1390	2065	-79 296 370
ATOM 1037 C		138 21.903			
ANISOU 1037 C			19.525	37.505	1.000 13.61
TMT200 103 / C	LEU	138 1305	2026	1840	-65 174 5

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ATOM 1038 O LEU 138 22.695 18.760 36.920 1.000 14.97 ANISOU 1038 O LEU 138 1125 2247 2313 105 234 178 1039 N ARG 139 22.184 20.816 37.614 1.000 13.26 ANISOU 1039 N ARG 139 1432 2046 1561 -155 219 3 ATOM 1040 CA ARG 139 23.397 21.372 37.085 1.000 14.71 -155 219 317 ANISOU 1040 CA ARG 139 1648 1941 2000 -27 502 447 1041 C ARG 139 1446 1941 2000 -27 502 447
1041 C ARG 139 24.636 20.815 37.775 1.000 15.16
1041 C ARG 139 1425 2101 2235 -158 324 116
1042 O ARG 139 25.650 20.495 37.166 1.000 18.15
1042 O ARG 139 1628 2581 2688 18 612 3 3 9
1043 CB ARG 139 23.394 22.926 37.206 1.000 19.67 ATOM ANISOU 1041 C ATOM ANISOU 1042 O ATOM ATOM 1043 CB ARG 139 1749 1923 3803 -196 186 252 ATOM 1044 CG ARG 139 24.418 23.487 36.237 1.000 28.66 ANISOU 1044 CG ARG 139 3924 2584 4383 -2305 882 -563 ATOM 1045 CD ARG 139 24.245 24.997 36.111 1.000 39.58 ANISOU 1045 CD ARG 139 6801 2389 5849 -3273 119 -306 ATOM 1046 NE ARG 139 24.910 25.660 37.210 1.000 47.91 ANISOU 1046 NE ARG 139 9548 2435 6222 -2157 -1331 ATOM 1047 CZ ARG 139 24.493 26.682 37.928 1.000 45.42 -2157 -1331 -708 ANISOU 1047 CZ ARG 139 6941 4516 5802 -882 -2118 ATOM 1048 NH1 ARG 139 23.316 27.273 37.722 1.000 64.33 -882 -2118 -1238 ANISOU 1048 NH1 ARG 139 7248 8153 9039 93 - 2965 - 980 ATOM 1049 NH2 ARG 139 7248 8153 9039 93 -2965 -98 ATOM 1049 NH2 ARG 139 25.309 27.109 38.888 1.000 32.62 ANISOU 1049 NH2 ARG 139 5020 4758 2616 -2746 590 1 ATOM 1050 N ALA 140 24.562 20.684 39.096 1.000 14.85 -2746 590 167 ATOM 1050 N ALA 140 24.562 20.684 39.096 1.000 14.85

ANISOU 1050 N ALA 140 1287 2204 2151 -517 -26 -4

ATOM 1051 CA ALA 140 25.730 20.257 39.856 1.000 15.80

ANISOU 1051 CA ALA 140 989 2649 2366 -309 -9 -401

ATOM 1052 CB ALA 140 25.444 20.442 41.330 1.000 19.36

ANISOU 1052 CB ALA 140 2685 2447 2222 243 -435 -4

ATOM 1053 C ALA 140 26.111 18.806 39.584 1.000 16.86

ANISOU 1053 C ALA 140 25.55 2795 2054 12 -186 -45

ATOM 1054 O ALA 140 27.258 18.403 39.796 1.000 18.90

ANISOU 1054 O ALA 140 1538 2686 2958 -21 60 145

ATOM 1055 N THR 141 25.147 18.025 39.098 1.000 17.53

ANISOU 1055 N THR 141 25.147 18.025 39.098 1.000 17.53

ANISOU 1056 CA THR 141 25.340 16.625 38.765 1.000 15.59

ANISOU 1056 CA THR 141 225.340 16.625 38.765 1.000 15.59

ANISOU 1057 CB THR 141 1238 2200 2172 155 282 30

ATOM 1058 OG1 THR 141 1238 2200 2172 155 282 30

ATOM 1058 OG1 THR 141 1249 1565 1926 -31 295 47

ANISOU 1058 OG1 THR 141 1249 1565 1926 -31 295 47

ANISOU 1059 CG2 THR 141 1394 2077 2160 135 -47 15

ATOM 1059 CG2 THR 141 1394 2077 2160 135 -47 15

ATOM 1060 C THR 141 1394 2077 2160 135 -47 15

ATOM 1060 C THR 141 1394 2077 2160 135 -47 15

ATOM 1060 C THR 141 25.423 16.374 37.257 1.000 16.11 -517 -26 -46 243 -435 - 480 12 - 186 - 458 60 1 4 5 -528 218 -108 -192 -95 291 282 301 295 476 -47 177 THR 141 25.423 16.374 37.257 1.000 16.11 THR 141 1732 2046 2343 303 583 3 1060 C ANISOU 1060 C 2343 3 2 5 THR 141 25.432 15.235 36.778 1.000 17.55 THR 141 1991 2104 2573 237 555 2 1061 0 ATOM ANISOU 1061 O 555 249 1062 N GLY 142 25.474 17.416 36.446 1.000 17.74 MOTA ANISOU 1062 N GLY 142 2127 2197 260 501 2416 303 1063 CA GLY 142 25.611 17.263 34.987 1.000 17.32 ATOM ANISOU 1063 CA GLY 142 1642 2494 2447 -160 453 517 1064 C GLY 142 24.426 16.556 34.358 1.000 16.37 ATOM ANISOU 1064 C ATOM 1065 O ANISOU 1065 O GLY 142 1619 1893 2710 261 472 4 2 GLY 142 24.654 15.824 33.379 1.000 18.43 GLY 142 2243 2558 2201 57 798 163 THR 143 23.232 16.738 34.907 1.000 13.99 THR 143 1531 1429 2356 83 430 3 5 0 ATOM 1066 N ANISOU 1066 N 1067 CA THR 143 22.049 16.003 34.472 1.000 14.69 ATOM ANISOU 1067 CA THR 143 1768 1591 2223 8 342 9 3 ATOM 1068 CB THR 143 21.208 15.584 35.700 1.000 15.52

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ANISOU 1068 CB THR 143 1457 1653 2785 55 419 5 2 9
ATOM 1069 OG1 THR 143 22.037 14.784 36.573 1.000 14.63
ANISOU 1069 OG1 THR 143 1296 1792 2471 52 434 3 6 9
        ANISOU 1068 CB THR 143 1457
ANTSOU 1069 0G1 THR 143 1296 1792 2471 52434369 ATOM 1070 CG2 THR 143 20.044 14.738 35.231 1.000 14.24 ANTSOU 1070 C THR 143 21.135 16.785 31.532 1.000 14.24 18.479 -131 ANTSOU 1071 C THR 143 1553 1708 20.44 128 479 -131 ANTSOU 1072 C THR 143 2374 1580 1995 315 486 5 5 ATOM 1073 N GLU 144 20.928 16.279 32.322 1.000 15.65 ANTSOU 1073 N GLU 144 1734 1580 1995 315 486 5 5 ATOM 1073 N GLU 144 1734 1904 2184 -156 260 -271 ANTSOU 1074 CA GLU 144 18.774 15.693 31.923 1.000 15.32 ANTSOU 1074 CA GLU 144 18.774 15.693 31.392 1.000 15.32 ANTSOU 1075 C GLU 144 18.774 15.693 31.392 1.000 15.32 ANTSOU 1075 C GLU 144 18.774 15.693 31.392 1.000 15.32 ANTSOU 1075 C GLU 144 18.774 15.693 31.392 1.000 16.84 ANTSOU 1075 C GLU 144 18.774 15.693 31.392 1.000 16.84 ANTSOU 1075 C GLU 144 18.792 14.631 30.680 1.000 16.71 ANTSOU 1076 C GLU 144 170 ATOM 1076 C GLU 144 170 ATOM 1077 CB GLU 144 20.539 16.856 29.970 1.000 21.91 ANTSOU 1079 CD GLU 144 19.602 19.355 ANTSOU 1079 CD GLU 144 19.602 19.355 ANTSOU 1079 CD GLU 144 19.602 19.355 ANTSOU 1080 CEI GLU 144 19.602 19.355 ANTSOU 1080 CEI GLU 144 19.602 19.355 ANTSOU 1080 CEI GLU 144 18.766 18.798 27.367 1.000 21.91 ANTSOU 1080 CEI GLU 144 18.766 18.798 27.367 1.000 21.91 ANTSOU 1080 CEI GLU 144 18.766 18.798 27.367 1.000 21.91 ANTSOU 1080 CEI GLU 144 18.766 18.798 27.367 1.000 21.91 ANTSOU 1080 CEI GLU 144 18.766 18.798 27.367 1.000 21.91 ANTSOU 1080 CEI GLU 144 18.766 18.798 27.367 1.000 14.12 ANTSOU 1080 CEI GLU 144 18.766 18.798 27.367 1.000 14.12 ANTSOU 1080 CEI GLU 144 18.766 18.798 27.367 1.000 14.12 ANTSOU 1080 CEI GLU 144 18.766 18.798 27.367 1.000 14.20 ANTSOU 1080 N PRO 145 16.507 15.000 14.20 ANTSOU 1080 CEI GLU 144 18.766 18.798 27.367 1.000 14.20 ANTSOU 1080 CEI GLU 144 18.766 18.798 27.367 1.000 14.20 ANTSOU 1080 CEI GLU 144 18.766 18.798 27.367 1.000 14.20 ANTSOU 1080 CEI GLU 144 18.766 18.798 27.367 1.000 14.20 ANTSOU 1080 CEI GLU 144 18.766 18.798 27.367 1.000 14.20 ANTSOU 1080 CEI GLU 144 18.766 18.798 27.367 1.000 14.20 ANTSOU 1080 CEI GLU 144 18.766 18.798 27.367 1.000
        ATOM 1070 CG2 THR 143 20.044 14.738 35.231 1.000 14.24
ANISOU 1070 CG2 THR 143 1761 1981 1669 3 379 192
                              1092 UG ASP 146 4012 2450 3813 -720 -229 -8
1093 OD1 ASP 146 12.295 12.121 27.409 1.000 38.65
1093 OD1 ASP 146 3943 4880 5050
        ANISOU 1093 OD1 ASP 146 3943
                                                                                                                       4889
                                                                                                                                                   5852
                                                                                                                                                                             -595 -1282 -323
                            1094 OD2 ASP 146 14.091 11.311 26.466 1.000 39.95
        ATOM
       ANISOU 1094 OD2 ASP 146 6913
                                                                                                                       5052
                                                                                                                                                   3214
                                                                                                                                                                             160 -1182
       ATOM 1095 C ASP 146 13.860 14.441 28.552 1.000 16.65
ANISOU 1095 C ASP 146 2461 1904 1961 -128 580 -
                                                                                                                                                                             -128 580 - 40
                           1096 O ASP 146 13.041 14.605 29.457 1.000 15.67
        ATOM
       ANISOU 1096 O ASP 146 2110 1935 1908
                                                                                                                                                                            -334 381 -420
                           1097 N GLY 147 13.871 15.149 27.429 1.000 20.60
        ATOM
        ANISOU 1097 N
                                                             GLY 147 3484 2416 1927
                                                                                                                                                                            -26
                                                                                                                                                                                                419 129
                           1098 CA GLY 147 12.903 16.212 27.155 1.000 18.06
        ANISOU 1098 CA GLY 147 2771
                                                                                                                     2451
                                                                                                                                                1638
                                                                                                                                                                           -382 98 9 3
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GLY 147 13.361 17.574 27.609 1.000 18.73 GLY 147 2836 2195 2085 -524 143 5 ATOM 1099 C ANISOU 1099 C GLY 147 2836 2195 2085 -524 143 5 GLY 147 12.676 18.570 27.282 1.000 18.34 -524 143 527 MOTA 1100 0 GLY 147 2865 ANISOU 1100 O 2416 1687 -413 -72 389 1101 N GLY 148 14.498 17.634 28.316 1.000 16.35 J 1101 N GLY 148 2936 1506 1772 -157 142 8 1102 CA GLY 148 15.116 18.889 28.747 1.000 15.34 ATOM ANISOU 1101 N -157 142 8 8 ANISOU 1102 CA GLY 148 2723 1279 1829 55 450 - 26 1103 C GLY 148 14.768 19.339 30.144 1.000 12.97 MOTA ANISOU 1103 C GLY 148 2231 1416 1280 -93 -62 40 7

ANISOU 1104 O GLY 148 13.769 18.930 30.771 1.000 12.81

ANISOU 1105 N VAL 149 15.604 20.224 30.718 1.000 12.81

ANISOU 1105 N VAL 149 1815 1366 1686 155 -31 2 3 8

ATOM 1106 CA VAL 149 15.388 20.724 32.079 1.000 11.81

ANISOU 1106 CA VAL 149 1333 1390 1765 54 -92 1 2 9

ATOM 1107 CB VAL 149 1136 1696 1717 -100 246 1 2 4

ATOM 1108 CG1 VAL 149 16.594 21.636 32.480 1.000 11.97

ANISOU 1108 CG1 VAL 149 16.358 22.336 33.802 1.000 15.26

ANISOU 1108 CG1 VAL 149 1941 1922 1936 -195 55 -22 3

ATOM 1109 CG2 VAL 149 1231 2045 32.538 1.000 17.21

ANISOU 1109 CG2 VAL 149 1231 2045 32.538 1.000 17.21

ANISOU 1100 C VAL 149 14.101 21.482 32.280 1.000 11.32

ANISOU 1110 C VAL 149 13.378 21.218 33.253 1.000 12.35

ANISOU 1111 O VAL 149 13.375 21.482 32.280 1.000 12.35

ANISOU 1112 N GLU 150 13.752 22.463 31.460 1.000 11.96

ANISOU 1113 CA GLU 150 12.592 23.286 31.815 1.000 10.90

ANISOU 1113 CA GLU 150 12.592 23.286 31.815 1.000 17.60 ANISOU 1103 C GLY 148 2231 1416 1280 -93 -62 4 0 7 ANISOU 1113 CA GLU 150 1623 1359 1159 118 0 4 0 5 ATOM 1114 CB GLU 150 12.608 24.601 30.999 1.000 17.60 118 0 4 0 5 ANISOU 1114 CB GLU 150 12.608 24.601 30.999 1.000 17.60 ANISOU 1114 CB GLU 150 2530 1470 2687 181 -1619 0 7 ATOM 1115 CG GLU 150 13.811 25.488 31.314 1.000 17.86 ANISOU 1115 CG GLU 150 13.956 25.929 32.738 1.000 19.47 ANISOU 1116 CD GLU 150 3018 1353 3027 -97 -84 662 ATOM 1117 OE1 GLU 150 12.951 26.005 33.475 1.000 19.47 ANISOU 1117 OE1 GLU 150 3035 1512 2373 -178 -321 5 3 6 ATOM 1118 OE2 GLU 150 15.109 26.237 33.122 1.000 22.59 ANISOU 1118 OE2 GLU 150 2993 1664 3927 -38 -150 28 4 ATOM 1119 C GLU 150 11.277 22.533 31.705 1.000 12.22 ANISOU 1119 C GLU 150 1429 1540 1676 235 147 - 5 ATOM 1120 O GLU 150 1429 1540 1676 235 147 - 5 ATOM 1120 O GLU 150 1739 1474 1894 315 470 28 8 ATOM 1121 N ALA 151 11.118 21.625 30.742 1.000 13.44 ANISOU 1121 N ALA 151 1783 1255 1477 94 45 2 5 3 ATOM 1122 CA ALA 151 9.881 20.844 30.698 1.000 13.82 ANISOU 1123 CB ALA 151 9.789 20.094 29.390 1.000 14.89 ANISOU 1123 CB ALA 151 9.789 20.094 29.390 1.000 14.89 ANISOU 1124 C ALA 151 1448 1463 1920 93 41 4 2 4 ATOM 1124 C ALA 151 1448 1463 1920 93 41 4 2 4 ATOM 1125 O ALA 151 18.655 19.580 32.280 1.000 14.69 ANISOU 1125 O ALA 151 18.655 19.580 32.280 1.000 14.69 ANISOU 1114 CB GLU 150 2530 1470 2687 181 -161 9 0 7 1125 O ALA 151 8.655 19.580 32.280 1.000 14.69 MOTA ANISOU 1125 O ALA 151 1535 2114 1932 -242 204 -108 1126 N ATOM PHE 152 10.925 19.401 32.410 1.000 11.73 ANISOU 1126 N PHE 152 1598 1259 1598 120 1127 CA PHE 152 10.890 18.554 33.602 1.000 10.61 ATOM ANISOU 1127 CA PHE 152 1444 1061 1526 -33 34 1 6 0 ATOM 1128 CB PHE 152 12.293 17.981 33.820 1.000 10.23 ANISOU 1128 CB PHE 152 1317 1132 1437 -144 207 410 1129 CG PHE 152 12.517 17.187 35.095 1.000 10.36

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ANISOU	1129	CG	PHE	150	1388	1149	1399	-34 147 276
ATOM	1130							
				T 2 7	12.036	15.896	35.229	
ANISOU					1479	1047	1743	114 -103 5 6 6
ATOM	1131	CD2	PHE	152	13.229	17.701	36.154	1.000 11.21
ANISOU	1131	CD2	PHE		1489	1449	1319	85 174 1 5 1
ATOM	1132				12.252			
						15.163	36.380	1.000 10.80
ANISOU				152	1400	1234	1467	249 -111 3 7 3
ATOM	1133	CE2	PHE	152	13.431	16.992	37.341	1.000 11.82
ANISOU	1133	CE2	PHE		1709	1622	1160	-276 414 250
ATOM	1134		PHE	150	12.932	15.717		
							37.457	1.000 11.97
ANISOU			PHE		1651	1604	1293	-255 296 170
ATOM	1135		PHE	152	10.430	19.292	34.858	1.000 12.24
ANISOU	1135	С	PHE	152	1754	1168	1730	-10 339 8 4
ATOM		Ó	PHE		9.728	18.729		
							35.726	1.000 11.49
ANISOU			PHE		1672	1142	1550	200 109 277
MOTA	1137		LEU		10.809	20.575	34.997	1.000 11.86
ANISOU	1137	N	LEU	153	2030	1236	1240	-6 73 1 5 6
MOTA	1138	CA	LEU		10.532	21.386	36.155	1.000 11.99
ANISOU			LEU					
					1890	1229	1437	-165 307 8 5
ATOM	1139		LEU	T 5 3	11.654	22.420	36.353	1.000 12.81
ANISOU	1139	CB	LEU	153	1691	1381	1794	-72 97 - 40
ATOM	1140	CG	LEU	153	13.059	21.910	36.592	1.000 12.87
ANISOU			LEU		1762	1645		
ATOM	1141						1483	146 269 6 4
					14.027	23.081	36.611	1.000 15.99
ANISOU					1609	2006	2462	-49 450 -431
MOTA	1142	CD2	LEU	153	13.185	21.158	37.914	1.000 19.37
ANISOU	1142	CD2	LEU		3091	2462	1806	809 275 540
ATOM		С	LEU		9.179	22.084		
ANISOU				150	1700		36.123	1.000 12.96
			LEU		1728	1253	1943	-336 360 -43
ATOM	1144		LEU		8.709	22.506	37.193	1.000 13.24
ANISOU	1144	0	LEU	153	1617	1302	2109	-443 481 -182
ATOM	1145	N	ASP		8.568	22.203	34.955	1.000 13.29
ANISOU			ASP		1643			
						1457	1951	60 517 2 8 0
MOTA	1146	CA	ASP		7.195	22.671	34.764	1.000 14.21
ANISOU	1146	CA	ASP	154	1862	1255	2280	313 631 683
ATOM	1147	CB	ASP	154	6.995	23.269	33.373	1.000 18.38
ANISOU			ASP		2091	2156	2738	328 728 1475
ATOM	1148		ASP		5.534			
						23.367	32.929	1.000 22.95
ANISOU			ASP		2323	3543	2855	676 430 1501
ATOM	1149	OD1	ASP	1.54	4.685	23.607	33.820	1.000 20.85
ANISOU	1149	OD1	ASP		2164	2368	3389	895 478 1144
ATOM	1150	OD2	ACD	15/		23.254	31.702	1.000 24.33
ANISOU								
					2989	3146		228 48 1 1 2 8
ATOM	1151		ASP		6.294	21.455	34.985	1.000 11.22
UOZINA			ASP	154	1594	1403	1265	123 147 410
ATOM	1152	0	ASP		6.043	20.729	34.015	1.000 13.31
ANISOU			ASP		2143	1728		
ATOM	1153						1186	427 219 170
			CYS		5.891	21.220	36.233	1.000 9 . 9 1
ANISOU			CYS		1425	1098	1243	-76 186 2 7
MOTA	1154		CYS		5.446	19.881	36.627	1.000 9 . 4 1
ANISOU	1154	CA	CYS		1294	1168	1115	-13 154 1 7 2
ATOM	1155		CYS		6.635			
						19.171	37.269	1.000 10.64
ANISOU			CYS	T 2 2	1276	1015	1753	28 -51 -122
ATOM	1156	SG	CYS	155	7.316	19.819	38.797	1.000 12.01
ANISOU	1156	SG	CYS	155	1376	1554	1633	-195 -199 9 5
ATOM	1157		CYS		4.138	19.885	37.423	1.000 9.66
ANISOU			CYS					
ATOM	1158				1301	1355	1013	115 146 216
			CYS	155	3.215	20.645	37.064	1.000 11.61
ANISOU			CYS		1349	1386	1676	130 116 294
ATOM	1159		GLU	156	4.021	19.033	38.442	1.000 10.26
ANISOU	1159	N	GLU		1263	1495	1139	-29 168 2 9 9
				-		-		

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ATOM 1160 CA GLU 156 2.778 18.787 39.173 1.00

ANISOU 1160 CA GLU 156 998 1160 1278 -76 -37 2 3 6

ATOM 1161 CB GLU 156 2.300 17.391 38.772 1.000 11.63

ANISOU 1161 CB GLU 156 1187 1348 1885 -67 -135 -1

TOM 1162 CG GLU 156 1.841 17.282 37.326 1.000 14.29

1162 CG GLU 156 1.841 17.282 37.326 1.000 14.29

17.949 37.039 1.000 17.90

-365 -686 1 -67 -135 -190 -628 -507 5 0 -365 -686 1 3 7 1164 OE1 GLU 156 -0.220 18.241 38.024 1.000 19.17 ANISOU 1164 OE1 GLU 156 1429 2973 -632 -270 2 5 3 2884 1165 OE2 GLU 156 0.136 18.198 35.858 1.000 22.03 ATOM ANISOU 1165 OE2 GLU 156 2449 3269 2653 -243 -721 9 2 4 ATOM 1166 C GLU 156 2.961 18.942 40.677 1.000 9.21 ANISOU 1166 C GLU 156 1166 1135 1197 -26 239 1 -26 239 183 ATOM 1167 O ANISOU 1167 O GLU 156 2.828 17.997 41.476 1.000 11.22 GLU 156 1631 1199 1434 103 162 4 PRO 157 3.337 20.158 41.118 1.000 10.29 103 162 431 ATOM 1168 N ANISOU 1168 N ATOM 1168 N PRO 157 3.337 20.158 41.118 1.000 10.29
ANISOU 1168 N PRO 157 1329 1201 1381 -109 21 1 2 3
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ANISOU 1171 CB PRO 157 1832 1567 1330 -397 20 5 8
ATOM 1172 CG PRO 157 3.475 22.471 41.429 1.000 10.44
ANISOU 1172 CG PRO 157 1469 1259 1237 -388 166 -19
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ANISOU 1177 CB LEU 158 1280 1447 1464 -251 99 9 3
ATOM 1178 CG LEU 158 0.111 18.239 47.155 1.000 12.01
ANISOU 1178 CG LEU 158 1271 1497 1795 -303 241 12
ATOM 1179 CD1 LEU 158 -1.212 18.826 46.736 1.000 16.21
ANISOU 1179 CD1 LEU 158 1224 2249 2685 -111 41 -23
ATOM 1180 CD2 LEU 158 -0.086 16.736 47.397 1.000 17.17
ANISOU 1180 CD2 LEU 158 2656 1542 2325 -254 1273 17
ATOM 1181 C LEU 158 1.997 20.626 47.048 1.000 11.22
ANISOU 1181 C LEU 158 1496 1366 1402 110 -304 5
ATOM 1182 O LEU 158 3.056 20.201 47.539 1.000 11.28
ANISOU 1182 O LEU 158 1283 1368 1635 20 -262 7 5
ATOM 1183 N LEU 159 1.234 21.599 47.548 1.000 10.86
ANISOU 1183 N LEU 159 1.234 21.599 47.548 1.000 10.86
ANISOU 1183 N LEU 159 1.234 21.599 47.548 1.000 10.86
ANISOU 1184 CA LEU 159 1.540 22.278 48.797 1.000 11.62
ANISOU 1184 CA LEU 159 1.540 22.278 48.797 1.000 11.62
ANISOU 1184 CA LEU 159 1.494 23.802 48.640 1.000 12.44 1177 CB LEU 158 1.152 18.482 46.078 1.000 11.03 ATOM -303 241 128 -111 41 - 239 -254 1273 1 7 4 68 - 180 - 70 -68 -180 1185 CB LEU 159 1.494 1185 CB LEU 159 1624 ATOM 23.802 48.640 1.000 12.44 ANISOU 1185 CB LEU 159 1624 -209 -73 -33 1747 1354 1186 CG LEU 159 1.633 24.635 49.934 1.000 12.83 ANISOU 1186 CG LEU 159 1600 246 -54 -215 1698 1576 ATOM 1187 CD1 LEU 159 2.947 ANISOU 1187 CD1 LEU 159 2019 24.435 50.651 1.000 14.28 2250 1158 177 -292 1 0 4 1188 CD2 LEU 159 1.442 ATOM 26.134 49.640 1.000 13.33 ANISOU 1188 CD2 LEU 159 1802 1721 1543 87 -87 - 20 ATOM 1189 C LEU 159 0.537 21.846 49.868 1.000 11.24 ANISOU 1189 C LEU 159 1393 1474 1404 -174 -9 -2711190 0 ATOM LEU 159 -0.665 21.940 49.620 1.000 13.70

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                                             LEU 159 1354
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                                                                                                                   1457 -328 34 - 269
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ANISOU 1191 N ARG 160 1737 2569 1239 -390 -128 -2

ATOM 1192 CA ARG 160 0.158 21.030 52.153 1.000 13.94

ANISOU 1192 CA ARG 160 1265 2631 1402 157 -137 9
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                     1194 CG ARG 160 -0.423 18.661 51.252 1.000 25.12
J 1194 CG ARG 160 3451 2902 3191 -653 -787 2
      ANISOU 1194 CG ARG 160 3451
                                                                                                                                        -653 -787 2 3
                      1195 CD ARG 160 -0.765 17.301 51.831 1.000 31.98
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     ANISOU 1195 CD ARG 160 4825 3598
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                                                                                                                                        -1994 -905 3 2 1
     ATOM 1196 NE ARG 160 -1.284 16.322 50.896 1.000 26.15
ANISOU 1196 NE ARG 160 3392 2957 3587 -739 -1056
ATOM 1196 NE ARG 160 -1.284 16.322 50.896 1.000 26.15

ANISOU 1197 CZ ARG 160 -0.970 15.044 50.779 1.000 25.30

ANISOU 1197 CZ ARG 160 -0.970 15.044 50.779 1.000 25.30

ANISOU 1198 NH1 ARG 160 -0.063 14.433 51.552 1.000 31.26

ANISOU 1198 NH1 ARG 160 -0.063 14.433 51.552 1.000 31.26

ANISOU 1199 NH2 ARG 160 -1.572 14.308 49.850 1.000 28.82

ANISOU 1199 NH2 ARG 160 0.649 21.669 53.447 1.000 15.12

ANISOU 1200 C ARG 160 1649 2863 1232 104 -66 1.25

ATOM 1201 O ARG 160 1.804 21.556 53.863 1.000 17.09

ANISOU 1201 O ARG 160 1.291 3411 1791 -400 74 -8.12

ATOM 1202 N PHE 161 -0.258 22.369 54.114 1.000 14.95

ANISOU 1202 N PHE 161 -0.258 22.369 54.114 1.000 14.95

ANISOU 1203 CA PHE 161 -0.036 22.949 55.427 1.000 13.27

ANISOU 1203 CA PHE 161 -0.587 24.381 55.472 1.000 13.27

ANISOU 1204 CB PHE 161 -0.587 24.381 55.472 1.000 16.82

ANISOU 1205 CG PHE 161 -0.317 25.109 56.771 1.000 22.56

ATOM 1206 CD1 PHE 161 -1.175 25.010 57.849 1.000 26.03

ANISOU 1207 CD2 PHE 161 3353 2919 3620 267 1106 -702

ATOM 1208 CE1 PHE 161 -0.943 25.666 59.051 1.000 30.50
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                        1208 CE1 PHE 161 -0.943 25.660 59.051 1.000 30.50
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                                                                                                                                        -972 1456 - 620
                                                                                                                                        -129 281 -1127
                                                                                                                                        -152 774 -677
                                                                                                                                        -334 -277 -240
                                                                                                                                        -744 -399 4 7 5
                                                                                                                                         -937 -523 7 7
                                                                                                                                        -519 -266 7 6
                                                                                                                                        -603 -186 - 76
                      1217 CB ARG 162 0.081
                                                                                                                                         -771 -42 -160
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                                                                                               19.374 58.458 1.000 21.99
      ANISOU 1217 CB ARG 162 3309
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                                                                                                                                                         655 280
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      ATOM
      ANISOU 1219 CD ARG 162 3106
                                                                                               2221
                                                                                                                     4495
                                                                                                                                        418
                                                                                                                                                       -2 2 3 9
                     1220 NE
                                                             162 -0.943 15.916 59.698 1.000 28.83
      ATOM
                                                 ARG
      ANISOU 1220 NE
                                                 ARG 162 4379 2437
                                                                                                                    4139
                                                                                                                                        -181 332 -177
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ATOM

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ATOM 1221 CZ ARG 162 -0.642 14.638 59.879 1.000 27.99 ANISOU 1221 CZ ARG 162 4271 2497 3868 -179 962 8 ANISOU 1221 CZ ARG 162 4271 2497 3868 -179 962 8
ATOM 1222 NH1 ARG 162 0.429 14.119 59.273 1.000 26.61
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ATOM 1223 NH2 ARG 162 -1.408 13.883 60.658 1.000 34.20
ANISOU 1223 NH2 ARG 162 3807 3522 5663 -986 702 7 -179 962 8 4 -126 - 268 -986 702 780 1224 N TYR 163 -1.570 21.296 60.622 1.000 16.77 MOTA TYR 163 1803 ANISOU 1224 N 2865 1705 -484 -1948 4 1225 CA TYR 163 -1.627 21.749 61.997 1.000 16.73 ATOM ANISOU 1225 CA TYR 163 1819 2770 1766 -692 -51 4 0 1226 CB TYR 163 -2.712 22.804 62.116 1.000 18.99 ANISOU 1226 CB TYR 163 2479 2560 2175 -427 -303 -2141227 CG TYR 163 -3.173 23.206 63.488 1.000 23.52 ANISOU 1227 CG TYR 163 2573 3821 2544 -16 -335 - 868 1228 CD1 TYR 163 -2.316 23.848 64.367 1.000 31.80 ANISOU 1228 CD1 TYR 163 3613 5005 3466 -1151 304 -2338 1229 CE1 TYR 163 -2.731 24.222 65.625 1.000 40.74 ATOM ANISOU 1229 CE1 TYR 163 5855 5676 3950 -1906 976 -3116 1230 CD2 TYR 163 -4.459 22.965 63.931 1.000 32.55 ATOM ANISOU 1230 CD2 TYR 163 3307 5654 3408 -1066 639 -2340 ATOM 1231 CE2 TYR 163 -4.902 23.332 65.189 1.000 42.99 163 5626 6630 4080 -2352 1989 -163 -4.017 23.960 66.025 1.000 42.52 ANISOU 1231 CE2 TYR -2352 1989 -2949 ATOM 1232 CZ TYR ANISOU 1232 CZ 163 6281 5799 4075 -1721 1943 -3714 163 -4.380 24.351 67.274 1.000 48.87 TYR ATOM 1233 OH TYR ANISOU 1233 OH TYR ATOM 1234 C TYR ANISOU 1234 C TYR 1235 0 ATOMTYR ANISOU 1235 O TYR ATOM 1236 N PHE ANISOU 1236 N PHE1237 CA PHE 164 -1.340 19.381 64.984 1.000 23.44 ATOM ANISOU 1237 CA PHE 164 4176 2692 2038 -727 -669 2 ATOM 1238 CB PHE 164 -0.073 18.617 65.327 1.000 26.02 -727 -669 2 1 9 ANISOU 1238 CB PHE 164 4594 2824 2470 -459 -822 3 ATOM 1239 CG PHE 164 0.407 17.669 64.231 1.000 29.00 -459 -822 3 7 9 ANISOU 1239 CG PHE 164 4118 3639 3263 -518 -427 - 254 1240 CD1 PHE 164 1.224 18.118 63.205 1.000 27.11 ATOM ANISOU 1240 CD1 PHE 164 3040 4013 3249 -198 -821 4 ATOM 1241 CD2 PHE 164 3040 4013 3249 -198 -821 4
ATOM 1241 CD2 PHE 164 0.051 16.332 64.240 1.000 28.37
ANISOU 1241 CD2 PHE 164 3935 3139 3704 472 30 - 64
ATOM 1242 CE1 PHE 164 1.657 17.248 62.223 1.000 28.13
ANISOU 1242 CE1 PHE 164 2730 3926 4034 -43 -229 6
ATOM 1243 CE2 PHE 164 0.459 15.464 63.250 1.000 31.71
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ATOM 1244 CZ PHE 164 1.276 15.924 62.234 1.000 30.26
ANISOU 1244 CZ PHE 164 3827 3808 3862 0 300 126 30 - 64 -293 657 -383 164 3827 3808 3862 0 300 1 2 6 164 -1.775 20.160 66.228 1.000 24.65 ANISOU 1244 CZ PHE 164 3827 1245 C ATOM PHE ANISOU 1245 C PHE 164 3541 4049 1777 -1025 -455 3 7 164 -0.889 20.713 66.885 1.000 25.54 ATOM 1246 0 PHE ANISOU 1246 O PHE 164 3520 4167 2019 -921 -440 -257PRO 165 -3.058 20.293 66.527 1.000 32.24 ATOM 1247 N ANISOU 1247 N PRO 165 3641 5095 3513 -1894 266 -680 1248 CA PRO 165 -3.486 21.012 67.720 1.000 32.98 MOTA ANISOU 1248 CA PRO 165 3570 5737 -1271 397 - 322 3225 165 -2.854 20.429 ATOM 1249 C PRO 68.986 1.000 38.48 ANISOU 1249 C PRO 165 4355 6808 3457 -1872 40 3 4 3 1250 O PRO 165 -2.551 19.230 69.034 1.000 53.87 ANISOU 1250 O PRO 7012 165 9948 3507 -959 692 1750

1251 CB PRO 165 -5.001 20.820 67.769 1.000 37.76

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	- 131 -		
	RO 165 3640 6479		380 - 717
	RO 165 -5.417 20.04		
	RO 165 3341 6449		-349 - 398
		6 65.734 1.000	
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	EU 178 4.994 9.11	66.116 1.000	
	EU 178 3397 3170		1344 4 0 1
	EU 178 5.882 8.53		
	EU 178 3497 3245		752 -620
	EU 178 7.245 7.94	65.348 1.000	29.43
	EU 178 3557 2950		371 - 979
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ANISOU 1258 CD1 LI			810 - 790
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	EU 178 2.845 9.35		39.60
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	RG 179 3.231 11.9		
	RG 179 1860 3289		
	RG 179 3.297 11.5		
	RG 179 2158 2721 RG 179 2.295 11.6	4434 39 99 37 62.139 1.000	
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	RG 179 2.897 17.4		39.43
	RG 179 8420 3029		
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	MET 180 6.894 9.75		18.52
	MET 180 2237 2019	2781 -398	-79 5 2
	MET 180 5.041 11.6	46 60.136 1.000	22.64
	MET 180 2571 2321	3709 -197	-549 6 8 3
	MET 180 5.065 11.3		27.90
	MET 180 3918 3095	3588 -453	-654 9 1 3
	MET 180 4.945 12.8 MET 180 2936 2942	38 57.629 1.000 3626 -399	25.01 124 851
	MET 180 4.385 12.0		37.00
	MET 180 5917 3450	4690 -258	-2680 1204
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ANISOU 1281 N A	ALA 181 2144 2139		-558 2 9 9

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ATOM	1284		ALA		7.576	7.409	59.738	1.000 15.43
ANISOU			ALA		2223	1717	1925	-315 -369 4 3 2
ATOM	1285		ALA		7.458	8.198	58.783	1.000 15.49
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ATOM	1286		PRO		8.698	6.733	59.986	1.000 16.03
ANISOU			PRO		2517	1745	1829	32 - 78 5 3 1
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ANISOU	1287		PRO		2321	2908	2221	-210 -306 1 2 4 0
ATOM ANISOU			PRO PRO		9.865 2573	6.907 1336	59.076	1.000 14.78
ATOM	1289		PRO		10.914	5.948	1706 59.649	-101 -86 299 1.000 16.20
ANISOU			PRO		2570	1978	1607	170 -251 7 7
ATOM	1290		PRO		10.479	5.713	61.066	1.000 19.28
ANISOU	1290	CG	PRO		2301	3071	1952	-199 -245 1 0 0 1
ATOM	1291		PRO		9.541	6.571	57.627	1.000 14.90
ANISOU			PRO		2230	1658	1772	-421 -262 3 4 0
ATOM	1292		PRO		8.920	5.573	57.249	1.000 15.38
ANISOU			PRO		2301	1587	1957	-467 -482 5 3 9
ATOM ANISOU	1293		HIS HIS		9.969 1737	7.460 1312	56.730	1.000 12.28 -154 -284 1 5 6
ATOM	1294		HIS		9.733	7.354	1617 55.300	1.000 11.90
ANISOU			HIS		1413	1495	1614	-254 -351 3 5
ATOM	1295		HIS		8.300	7.824	54.922	1.000 12.43
ANISOU		CB	HIS		1399	1368	1957	-128 -241 1 1 2
MOTA	1296		HIS		8.168	9.314	55.089	1.000 11.36
ANISOU			HIS		1349	1369	1600	-367 -296 5 6
ATOM ANISOU	1297				8.259	10.374	54.249	1.000 12.03
ANISOU	1298				1684 7.989	1296 9.858	1589 56.339	-43 157 - 10 1.000 13.27
ANISOU	1298	NDI	HIS		1901	1439	1700	-65 267 193
ATOM	1299				7.943	11.187	56.244	1.000 12.43
ANISOU					1939	1490	1296	77 -244 150
ATOM	1300				8.101	11.515	54.992	1.000 11.04
ANISOU					1560	1437	1199	215 -232 4 8
ATOM	1301		HIS	183	10.749	8.176	54.515	1.000 12.27
ANISOU ATOM	1301		HIS HIS		1446 11.433	1639	1577	-303 -282 - 67
						9.032	55.064	1.000 12.94 -558 -292 1 5
ATOM	1303	N	TYR	184	10.849	7.907		1.000 10.61
ANISOU			TYR			1027	1552	-41 -380 1 1 0
ATOM	1304	CA	TYR			8.800	52.256	1.000 11.36
ANISOU			\mathbf{T} YR		1475	1104	1738	-71 -264 1 7 8
ATOM	1305		TYR		12.628	8.151	51.481	1.000 11.79
ANISOU			TYR		1631	8.151 1114 6.907	1734	-62 -197 3 4
ATOM ANISOU	1306		TYR TYR		12.368 1680	921 16		1.000 11.29
ATOM			TYR			5.659		5 -893 174 1.000 11.76
ANISOU					1663	927 18		8 -487 190
MOTA	1308	CE1	TYR		11.911	4.526		1.000 12.64
ANISOU	1308	CE1	TYR	184	1960	878 19	64 17	3 -40 182
ATOM			TYR		12.333	6.949	49.279	1.000 11.13
ANISOU					1252	1302	1674	
ATOM ANISOU	1210 1210	CE2	TYR		12.102	5.834		1.000 12.93
ANISOU	1311		TYR TYR		1944 11.898	1422 4.611	1546	49 - 384 7 3
ANISOU			TYR		1717	1304	1972	1.000 13.14 30 -611 6 7
ATOM	1312		TYR		11.663			1.000 15.45

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ANISOU 1312 OH TYR 184 2028
                                                  1471
                                                             2373
                                                                        42 - 476 - 247
 MOTA
           1313 C
                        TYR 184 10.447 9.390
                                                             51.314 1.000 11.50
 ANISOU 1313 C
                         TYR 184 1445
                                                  1215
                                                             1709
                                                                        -187 -201 3 4 8
                         TYR 184 9.362
 ATOM
           1314 0
                                                  8.797
                                                             51.089 1.000 11.75
 ANISOU 1314 O
                        TYR 184 1305
                                                  1308
                                                             1853
                                                                        -106 -171 4 2 7
           1315 N
 ATOM
                        ASP
                               185 10.784 10.557 50.743 1.000 10.79
 ANISOU 1315 N
                         ASP
                               185 1581
                                                  1069
                                                             1449
                                                                        -141 -132 1 1 8
           1316 CA ASP
                                                  11.218 49.815 1.000 9.10
 MOTA
                               185 9.861
 ANISOU 1316 CA ASP
                                                             1277
                               185 1089
                                                  1093
                                                                        -326 23 2 0 6
 ATOM
         1317 CB ASP
                               185 9.934
                                                  12.743 49.886 1.000 10.13
 ANISOU 1317 CB ASP
                               185 1427
                                                  1095
                                                             1327
                                                                        -298 -178 1 7 7
           1318 CG ASP
 ATOM
                               185 9.540
                                                  13.388 51.185 1.000 11.79
 ANISOU 1318 CG ASP
                               185 1797 1350
                                                             1333
                                                                        -250 -149 1 1
           1319 OD1 ASP
 ATOM
                               185 9.681
                                                14.638 51.278 1.000 13.79
 ANISOU 1319 OD1 ASP
                               185 2050 1316
                                                             1875
                                                                        135 -52 - 26
                                185 9.114
           1320 OD2 ASP
                                                12.755 52.189 1.000 13.31
 ANISOU 1320 OD2 ASP
                                185 1805
                                                  1848
                                                             1405
                                                                        -411 -63 105
           1321 C ASP 185 1805 1848 1405 -411 -63 1 (
1321 C ASP 185 10.098 10.759 48.371 1.000 9.44
1321 C ASP 185 1036 1150 1401 -309 -26 1 (
1322 O ASP 185 11.234 10.469 48.005 1.000 10.64
1322 O ASP 185 1167 1376 1500 -127 -35 -2
1323 N LEU 186 9.038 10.684 47.568 1.000 10.09
1323 N LEU 186 1211 1186 1437 -272 -177 - 9
1324 CA LEU 186 9.124 10.312 46.161 1.000 10.60
 ANISOU 1321 C
                                                                        -309 -26 100
 ATOM
 ANISOU 1322 O
                                                                        -127 -35 -206
ATOM
ANISOU 1323 N
                                                                        -272 -177 -58
ATOM
ANISOU 1324 CA LEU 186 1641
                                                  986 1401 -239 -52 -44
ATOM
           1325 CB LEU 186 8.030
                                                  9.295 45.798 1.000 11.32
                                                  929 1721 -111 17 -479
7.977 46.602 1.000 12.60
ANISOU 1325 CB LEU 186 1652
            1326 CG LEU 186 7.989
ATOM
ANISOU 1326 CG LEU 186 1408
                                                  1039
                                                             2340
                                                                        -263 -200 - 166
            1327 CD1 LEU 186 6.896 7.064
ATOM
                                                             46.028 1.000 16.64
ANISOU 1327 CD1 LEU 186 1900
                                                 1373
                                                             3049
                                                                        -634 -398 - 135
ATOM 1328 CD2 LEU 186 9.356 7.332 46.629 1.000 13.84
ANISOU 1328 CD2 LEU 186 1438 1245 2575 -155 443 28
ATOM 1329 C LEU 186 9.024 11.521 45.223 1.000 10.90
ANISOU 1329 C LEU 186 1327 1211 1603 -3 -451 164
ATOM 1330 O LEU 186 8.768 11.406 44.031 1.000 13.60
ANISOU 1330 O LEU 186 2067 1608 1494 -211 -321 10
ATOM 1331 N SER 187 9.264 12.705 45.734 1.000 10.71
ANISOU 1331 N SER 187 1546 1129 1393 -76 -282 31
ATOM 1332 CA SER 187 9.401 13.943 44.998 1.000 10.49
ANISOU 1332 CA SER 187 9.401 13.943 44.998 1.000 10.49
ANISOU 1333 CB SER 187 1427 1191 1370 195 -107 48
ATOM 1333 CB SER 187 9.221 15.103 46.002 1.000 10.56
ANISOU 1333 CB SER 187 1105 1048 1857 298 161 53
ATOM 1334 OG SER 187 10.430 14.918 46.726 1.000 13.01
ANISOU 1334 OG SER 187 10.430 14.918 46.726 1.000 13.01
ANISOU 1335 C SER 187 10.774 14.062 44.336 1.000 10.47
ANISOU 1335 C SER 187 10.774 14.062 44.336 1.000 10.47
ANISOU 1335 C SER 187 1447 862 1669 135 -3 145
ATOM 1336 O SER 187 11.684 13.246 44.513 1.000 10.54
ANISOU 1336 O SER 187 11.684 13.246 44.513 1.000 10.54
           1328 CD2 LEU 186 9.356 7.332
 ATOM
                                                             46.629 1.000 13.84
                                                                        -155 443 283
                                                                         -211 -321 1 0 3
                                                                               -282 3 1 8
                                                                               -107 4 8 8
                                                                               161 532
                                                                        -132 -295 2 0 1
                                187 1577
 ANISOU 1336 O
                         SER
                                                   799 1629
                                                                    183
                                                                            -91 - 77
                                188 10.962 15.095 43.502 1.000 9.78
188 1419 978 1318 147 44 7 4
            1337 N
 ATOM
                         MET
 ANISOU 1337 N
                         MET
 MOTA
            1338 CA MET
                                188 12.267 15.584 43.065 1.000 9.94
 ANISOU 1338 CA MET
                                188 1394
                                                   942 1441 182 58 3 7
 ATOM
            1339 CB MET
                                188 12.128 16.543 41.891 1.000 10.89
 ANISOU 1339 CB MET 188 1523
                                                   840 1774 98 48 2 2 7
 MOTA
           1340 CG MET 188 13.385 17.258 41.470 1.000 11.40
 ANISOU 1340 CG MET 188 1403
                                                   1172
                                                              1756
                                                                         46 -51 2 1 4
            1341 SD MET 188 14.687 16.134 40.891 1.000 12.71
 ATOM
 ANISOU 1341 SD
                       MET
                               188 1619
                                                  1272
                                                              1940
                                                                         139 137 198
  MOTA
            1342 CE
                        MET
                               188 16.061 17.267 40.790 1.000 13.86
  ANISOU 1342 CE
                        MET
                                 188 1862
                                                   1399
                                                              2003
                                                                         -2911 - 90
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- 134 -1343 C MET 188 12.946 16.217 44.291 1.000 12.13 ANISOU 1343 C MET 188 1325 1586 1698 169 -18 -285 MET 188 13.971 15.727 44.804 1.000 11.52 1344 0 ANISOU 1344 O MET 188 1288 1553 1535 144 132 8 7 1345 N VAL 189 12.362 17.290 44.838 1.000 10.00 1345 N VAL 189 1290 1217 1292 53 -175 6 ANISOU 1345 N VAL 189 1290 ATOM 1346 CA VAL 189 12.745 17.894 46.099 1.000 9.70 ANISOU 1346 CA VAL 189 1209 1057 1420 -212 -45 1347 CB VAL 189 13.618 19.154 45.979 1.000 9.97 MOTA ANISOU 1347 CB VAL 189 1288 1103 1398 -238 129 189 ATOM 1348 CG1 VAL 189 14.953 18.837 45.266 1.000 13.45 ANISOU 1349 CG2 VAL 189 12.899 20.289 45.264 1.000 12.24 ANISOU 1349 CG2 VAL 189 1715 1242 1693 -25 150 29 ATOM 1350 C VAL 189 11.469 18.245 46.871 1.000 10.10 ANISOU 1350 C VAL 189 10.405 18.399 46.250 1.000 9.53 ANISOU 1351 O VAL 189 1153 1249 1217 -222 -190 8 ATOM 1352 N THR 190 11.609 18.327 48.187 1.000 8.66 ANISOU 1352 N THR 190 1273 894 1123 15 -202 127 ATOM 1353 CA THR 190 10.565 18.771 49.091 1.000 9.64 ANISOU 1354 CB THR 190 10.194 17.699 50.132 1.000 10.69 ANISOU 1354 CB THR 190 1231 1196 1635 -300 121 -9 ATOM 1355 OG1 THR 190 9.662 16.586 49.501 1.000 12.45 ANISOU 1355 OG1 THR 190 1333 1341 2055 -140 -258 -44 ANISOU 1350 THR 190 1333 1341 2055 -140 -258 -44 ANISOU 1350 THR 190 1333 1341 2055 -140 -1348 CG1 VAL 189 14.953 18.837 45.266 1.000 13.45 ATOM -236 390 143 -25 150 295 -456 -156 - 73 ANISOU 1353 CA THR -11 -228 - 9 9 MOTAANISOU 1354 CB THR -300 121 -54ATOM ANISOU 1355 OG1 THR 190 1333 1341 2055 -140 -258 -18.131 51.019 1.000 13.59 -140 -258 - 48 1356 CG2 THR 190 9.038 ATOM ANISOU 1356 CG2 THR 190 1121 1356 CG2 THR 190 1121 2222 1821 -272 151 - 1357 C THR 190 11.058 19.976 49.891 1.000 9.23 2222 -272 151 -195ATOM ANISOU 1357 C THR 190 1257 1096 1152 **-**102 **-**336 **-** 49 THR 190 12.149 19.867 50.447 1.000 10.54 1358 0 ATOM ANISOU 1358 O THR 190 1322 1292 1390 -5 -359 -122 LEU 191 10.313 21.064 49.978 1.000 10.23 ATOM 1359 N ANISOU 1359 N 1359 N LEU 191 1319 1167 1401 -71 -177 -1360 CA LEU 191 10.691 22.241 50.770 1.000 10.19 -71 -177 -133 ATOM 1360 CA LEU 191 10.691 22.241 50.770 1.000 10.19
ANISOU 1360 CA LEU 191 1259 1176 1438 0 -294 -14
ATOM 1361 CB LEU 191 10.604 23.511 49.910 1.000 11.52
ANISOU 1361 CB LEU 191 1203 1185 1990 -118 -601 3
ATOM 1362 CG LEU 191 11.897 23.898 49.167 1.000 13.23
ANISOU 1362 CG LEU 191 1898 1710 1419 -391 -358 9
ATOM 1363 CD1 LEU 191 12.333 22.794 48.218 1.000 15.25
ANISOU 1363 CD1 LEU 191 1685 2018 2091 -476 -214 -3
ATOM 1364 CD2 LEU 191 11.717 25.231 48.448 1.000 17.46
ANISOU 1364 CD2 LEU 191 2310 2044 2281 -14 17 6 0 4
ATOM 1365 C LEU 191 9.798 22.328 52.006 1.000 11.93
ANISOU 1366 O LEU 191 1275 1677 1579 56 -190 -37
ATOM 1366 O LEU 191 1276 2173 1676 1 -192 -60
ANISOU 1366 N ILE 192 10.394 22.483 53.190 1.000 11.06 ATOM 0 - 294 - 142-118 -601 3 2 -391 -358 9 7 -476 -214 -30517 6 0 4 56 -190 - 372 LEU 191 1276 2173 1676 1 -192 -601 ILE 192 10.394 22.483 53.190 1.000 11.06 1367 N 192 1115 ANISOU 1367 N ILE 192 1112 192 9.671 22.53 1071 1638 1487 -111 -92 -108 1368 CA ILE 22.539 54.443 1.000 11.13 ANISOU 1368 CA ILE 1521 11 -173 -149 ATOM 1369 CB ILE 192 9.927 21.304 55.330 1.000 12.94 1586 ANISOU 1369 CB ILE 192 2099 1232 -65 -9 -233 1370 CG2 ILE 192 9.221 21.428 56.673 1.000 16.06 ANISOU 1370 CG2 ILE 192 2479 1983 1641 -206 426 -215 1371 CG1 ILE 192 9.512 20.028 54.590 1.000 15.51 ANISOU 1371 CG1 ILE 192 2633 1658 1601 -400 - 48 - 1751372 CD1 ILE 18.765 55.339 1.000 25.71 192 9.845 ANISOU 1372 CD1 ILE 192 5869 -175 -1566 -301 1608 2290 1373 C ILE 192 9.966 23.809 55.253 1.000 11.47

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ANISOU 1373 C ILE 192 1330 1603 1427 -4 -222 -12
ATOM 1374 O ILE 192 11.123 24.106 55.567 1.000 13.33
ANISOU 1374 O ILE 192 1344 1738 1981 -96 -289 -2
ATOM 1375 N GLN 193 8.904 24.525 55.602 1.000 15.78
ANISOU 1375 N GLN 193 1316 2462 2219 -64 -5 -97
ATOM 1376 CA GLN 193 8.987 25.653 56.533 1.000 14.56
ANISOU 1376 CA GLN 193 1582 1858 2091 212 -304 -5 -4 -222 -122 -289 - 219 -5 - 9 7 5 -304 - 5291377 CB GLN 193 8.449 ATOM 26.975 56.020 1.000 20.03 ANISOU 1377 CB GLN 193 2226 2203 3180 318 -329 1 4 2 1378 CG GLN 193 9.203 ATOM 27.684 54.914 1.000 23.86 ANISOU 1378 CG GLN 193 3399 2492 3174 313 45 2 8 0 1379 CD GLN 193 8.665 MOTA 29.079 54.675 1.000 22.92 ANISOU 1379 CD GLN 193 3250 2363 78 -477 2 0 5 3097 1380 OE1 GLN 193 7.603 29.292 54.099 1.000 27.68 ANISOU 1380 OE1 GLN 193 4175 3310 3031 552 -1214291381 NE2 GLN 193 9.411 30.075 55.134 1.000 27.01 ATOM ANISOU 1381 NE2 GLN 193 3187 2667 4408 -440 124 1 7 1382 C ATOM GLN 193 8.216 25.265 57.804 1.000 15.14 ANISOU 1382 C GLN 193 1945 1827 1982 136 -174 - 722
ATOM 1383 O GLN 193 7.147 24.662 57.714 1.000 27.80
ANISOU 1383 O GLN 193 2523 6225 1817 -1586 -592 2 3 5
ATOM 1384 N GLN 194 8.714 25.552 58.978 1.000 19.80
ANISOU 1384 N GLN 194 2994 2502 2025 -632 -752 3 3
ATOM 1385 CA GLN 194 8.100 25.080 60.213 1.000 22.89
ANISOU 1385 CA GLN 194 3961 2626 2110 493 -20 5 2
ATOM 1386 C GLN 194 7.763 26.236 61.141 1.000 27.79
ANISOU 1386 C GLN 194 4886 2757 2916 823 25 -262
ATOM 1387 O GLN 194 4886 2757 2916 823 25 -262
ATOM 1387 O GLN 194 4727 3168 3516 368 -259 -910
ANISOU 1388 CB GLN 194 9.086 24.170 60.950 1.000 23.97
ANISOU 1388 CB GLN 194 9.086 24.170 60.950 1.000 23.97
ANISOU 1389 CG GLN 194 9.398 22.835 60.314 1.000 21.94
ANISOU 1389 CG GLN 194 9.398 22.835 60.314 1.000 21.94 ANISOU 1382 C GLN 193 1945 1827 1982 136 -174 - 722 ATOM 1389 CG GLN 194 9.398 22.835 60.314 1.000 21.94 ANISOU 1389 CG GLN 194 2740 3238 2358 683 -182 -ATOM 1390 CD GLN 194 10.546 22.148 61.052 1.000 20.51 ANISOU 1390 CD GLN 194 2450 3433 1911 509 -321 -683 -182 - 10 509 -321 - 429 ATOM 1391 OE1 GLN 194 11.707 22.142 60.627 1.000 20.80 ANISOU 1391 OE1 GLN 194 2245 2996 2662 -171 -382 - $-171 \quad -382 \quad -681$ 1392 NE2 GLN 194 10.223 21.585 62.197 1.000 24.91 MOTA ANISOU 1392 NE2 GLN 194 2539 3902 3023 210 -365 760 THR 195 6.817 26.035 62.030 1.000 32.47 MOTA 1393 N ANISOU 1393 N THR 195 5716 2729 3891 1095 1056 - 616 1394 CA THR 195 6.588 26.708 63.282 1.000 35.83 MOTA ANISOU 1394 CA THR 195 6329 3539 3748 1011 999 -722 ATOM 1395 CB THR 195 5.263 27.492 63.357 1.000 37.50 ANISOU 1395 CB THR 195 5756 4304 4365 647 2095 - 1 ATOM 1396 OG1 THR 195 4.191 26.576 63.604 1.000 48.36 ANISOU 1396 OG1 THR 195 4.958 28.175 62.033 1.000 44.54 ANISOU 1397 CG2 THR 195 4.958 28.175 62.033 1.000 44.54 ANISOU 1397 CG2 THR 195 2944 7471 6510 -872 -963 62 ATOM 1398 C THR 195 6.590 25.684 64.429 1.000 48.86 ANISOU 1398 C THR 195 10133 4924 3508 -321 -1356 - ATOM 1399 O THR 195 6.122 24.544 64.293 1.000 64.12 ANISOU 1399 O THR 195 13267 4150 6945 -264 -4541 JATOM 1400 N PHE 201 12.035 21.374 72.205 1.000 71.12 ANISOU 1400 N PHE 201 13961 9034 4028 -5932 -1658 -MOTA 1395 CB THR 195 5.263 27.492 63.357 1.000 37.96 2095 - 1151 -806 2581 -1842 -872 -963 6 2 1 -321 -1356 -221 -264 -4541 1682 PHE 201 13961 9034 4028 -5932 -1658 -1741 1401 CA PHE 201 11.775 20.053 71.629 1.000 49.44 ATOM ANISOU 1401 CA PHE 201 7918 7543 3326 -3128 1317 -1488 1402 CB PHE 201 10.469 19.464 72.181 1.000 47.85 ANISOU 1402 CB 201 7119 PHE 6892 4168 -1869 1937 -1899 201 10.130 18.113 71.545 1.000 46.41 ATOM 1403 CG PHE ANISOU 1403 CG PHE 201 6643 6596 4396 -2038 1879 -1497

- 136 -ATOM 1404 CD1 PHE 201 10.738 16.954 71.991 1.000 50.03 ANISOU 1404 CD1 PHE 201 7982 6634 4393 -2326 1092 - 3400 1405 CD2 PHE 201 9.220 18.001 70.513 1.000 42.63 ANISOU 1405 CD2 PHE 201 5458 6427 4313 -1097 2449 - 2400 1406 CE1 PHE 201 10.434 15.739 71.417 1.000 49.95 ANISOU 1406 CE1 PHE 201 8275 6464 4240 -2047 227 - 5400 1407 CE2 PHE 201 8.901 16.783 69.934 1.000 41.38 ANISOU 1407 CE2 PHE 201 6016 5946 3762 -578 2006 -1400 1408 CZ PHE 201 9.515 15.636 70.392 1.000 44.74 -2326 1092 - 991 -1097 2449 - 2268 -2047 227 - 716 ATOM 1408 CZ PHE 201 6016 5946 3762 -578 2006 -1 ANISOU 1408 CZ PHE 201 9.515 15.636 70.392 1.000 44.74 ANISOU 1408 CZ PHE 201 7075 6261 3663 -1063 1020 -1 -578 2006 - 1844 -1063 1020 - 975 ATOM 1409 C PHE 201 11.722 20.110 70.107 1.000 42.42 ANISOU 1409 C PHE 201 6324 6442 3351 -1964 717 --1964 717 -1441 ATOM 1410 0 PHE 201 11.007 20.941 69.536 1.000 47.79 ANISOU 1410 0 PHE 201 9668 4400 4090 -762 691 -1433 CA GLN 205 14.288 14.143 62.574 1.000 12.76 ANISOU 1433 CA GLN 205 1777 1655 1419 43 - 347 - 113 GLN 205 14.622 13.434 61.260 1.000 11.12 ATOM 1434 C

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ANISOU 1434 C GLN 205 1412 1474 1338 49 -468 - 21 ATOM 1435 O GLN 205 13.707 12.927 60.606 1.000 13.97 ANISOU 1435 O GLN 205 1622 2235 1449 -293 -449 - 2 ATOM 1436 CB GLN 205 14.164 13.062 63.662 1.000 15.57 ANISOU 1436 CB GLN 205 2421 1925 1568 341 151 8 1338 49 - 468 - 21 -293 -449 -147 U 1437 CG GLN 205 3321 2286 1451 500 18.58 151 8 3 ATOM 689 -129 8 2 520 -499 - 570 ATOM 1439 OE1 GLN 205 16.206 13.717 65.549 1.000 29.12 ANISOU 1439 OE1 GLN 205 3350 3464 4251 14 -270 -18 14 -270 -1800 1440 NE2 GLN 205 14.840 15.356 66.378 1.000 23.01 ATOM 1440 NE2 GLN 205 14.840 15.356 66.378 1.000 23.01 ANISOU 1441 N ALA 206 15.893 13.401 60.893 1.000 12.63 ANISOU 1441 N ALA 206 15.893 13.401 60.893 1.000 12.63 ANISOU 1441 N ALA 206 16.335 1770 1506 -251 -234 - 6 ANISOU 1442 CA ALA 206 16.335 12.649 59.731 1.000 13.77 ANISOU 1443 CB ALA 206 16.693 13.519 58.528 1.000 16.34 ANISOU 1443 CB ALA 206 16.693 13.519 58.528 1.000 16.34 ANISOU 1444 C ALA 206 17.567 11.813 60.046 1.0015.92 ANISOU 1444 C ALA 206 17.567 11.813 60.046 1.0015.92 ANISOU 1444 C ALA 206 18.368 12.182 60.90 1.001 15.92 ANISOU 1444 C ALA 206 18.368 12.182 60.90 1.000 15.92 ANISOU 1444 C ALA 206 18.368 12.182 60.90 1.000 15.92 ANISOU 1444 C ALA 206 18.368 12.182 60.90 1.000 15.92 ANISOU 1444 C ALA 206 18.368 12.182 60.90 1.000 15.92 ANISOU 1444 C ALA 206 18.368 12.182 60.90 1.000 15.92 ANISOU 1444 C ALA 206 18.368 12.182 60.90 1.000 15.92 ANISOU 1444 C ALA 206 18.368 12.182 60.90 1.000 15.92 ANISOU 1444 C ALA 206 18.368 12.182 60.90 1.000 15.92 ANISOU 1444 C ALA 206 18.368 12.182 60.90 1.000 15.92 ANISOU 1444 C ALA 206 18.368 12.182 60.90 1.000 15.92 ANISOU 1444 C ALA 206 18.368 12.182 60.90 1.000 15.92 ANISOU 1444 C ALA 206 18.368 12.182 60.90 1.000 15.92 ANISOU 1444 C ALA 206 18.368 12.182 60.90 1.000 15.92 ANISOU 1445 C ALA 206 18.368 12.182 60.90 1.000 15.92 ANISOU 1445 C ALA 206 18.368 12.182 60.90 1.000 15.92 ANISOU 1445 C ALA 206 18.368 12.182 60.90 1.000 15.92 ANISOU 1450 CB GLU 207 19.948 10.953 57.503 1.000 16.23 ANISOU 1450 CB GLU 207 19.879 7.737 58.491 1.000 20.58 1 ANISOU 1450 CB GLU 207 19.879 7.737 58.492 1.000 30.08 ANISOU 1455 C G GLU 207 19.379 6.251 50.50 97 -948 -546 ANISOU 1455 C G GLU 207 19.379 6.251 50.90 97 -948 -546 ANISOU 1455 C G GLU 207 19.379 6.251 50.90 97 -948 -546 ANISOU 1455 C A VAL 208 22.376 11.593 88.90 1.000 16.97 ANISOU 1455 C A VAL 208 22.376 11.593 88.90 1.000 16.99 7 9.48 ANISOU 1455 C A VAL 208 22.376 11.593 88.90 1.000 17.77 ANISOU 1456 CA VAL 208 23.585 10.877 59.507 1.000 20.76 ANISOU 1456 C A VAL 208 23.585 10.877 59.507 1.000 20.76 ANISOU 1450 ANISOU 1440 NE2 GLN 205 3055 2465 3225 335 -592 - 140 1441 N ALA 206 15.893 13.401 60.893 1.000 12.63 ATOM 1179 -2099 -123 135 -2494 - 366 209 24.457 10.295 58.672 1.000 18.94 ATOM 1462 N GLY ANISOU 1462 N GLY 209 1764 2445 2989 -494 1 5 211 1463 CA GLY 209 25.558 9.508 59.194 1.000 24.01 ANISOU 1463 CA GLY 209 2171 3040 3910 -396 7 0 9 549 GLY 209 25.123 8.364 60.082 1.000 25.00 GLY 209 2874 3156 3470 1406 772 6 1464 C ANISOU 1464 C 1406 772 649

- 138 -1465 O GLY 209 25.850 7.934 60.991 1.000 35.98 ATOM GLY 209 4448 ANISOU 1465 O 3946 5279 1425 -426 1769 GLY 210 23.951 7.786 ATOM 1466 N 59.869 1.000 25.89 ANISOU 1466 N GLY 210 3802 2756 3278 523 899 749 1467 CA GLY 210 23.477 6.678 ATOM 60.671 1.000 26.43 ANISOU 1467 CA GLY 210 4479 2136 3427 1228 742 912 ATOM 1468 C GLY 210 22.885 7.025 ANISOU 1468 C GLY 210 5472 2099 62.016 1.000 28.45 3237 831 1029 1175 1469 O GLY 210 22.634 6.098 62.789 1.000 40.26 ATOM ANISOU 1469 O GLY 210 7322 2719 5256 1881 2759 2360 1470 N ALA 211 22.651 8.281 62.338 1.000 25.78 MOTA ANISOU 1470 N ALA 211 4671 2359 2763 1370 724 1197 1471 CA ALA 211 22.048 8.671 63.613 1.000 23.74 ATOM ANISOU 1471 CA ALA 211 2966 3156 2896 727 339 663 1472 CB ALA 211 23.093 9.333 64.496 1.000 29.57 ATOM ANISOU 1472 CB ALA 211 2957 4372 3906 834 -96 6 8

ATOM 1473 C ALA 211 20.900 9.626 63.360 1.000 21.19

ANISOU 1473 C ALA 211 3090 2611 2350 484 178 74

ATOM 1474 O ALA 211 20.936 10.381 62.399 1.000 23.91

ANISOU 1474 O ALA 211 3771 2659 2653 -30 -66 93

ATOM 1475 N PHE 212 19.889 9.629 64.204 1.000 19.88

ANISOU 1475 N PHE 212 2603 2577 2375 398 -128 37

ATOM 1476 CA PHE 212 18.814 10.613 64.130 1.000 19.13

ANISOU 1476 CA PHE 212 2581 2257 2432 284 -565 31

ATOM 1477 C PHE 212 19.320 12.006 64.489 1.000 20.00

ANISOU 1477 C PHE 212 19.893 12.230 65.569 1.000 21.10

ANISOU 1478 O PHE 212 19.893 12.230 65.569 1.000 21.10

ANISOU 1478 O PHE 212 2497 3558 1964 -391 -406 22

ATOM 1479 CB PHE 212 17.688 10.290 65.096 1.000 21.37

ANISOU 1479 CB PHE 212 17.688 10.290 65.096 1.000 21.37

ANISOU 1479 CB PHE 212 17.688 10.290 65.096 1.000 23.45

ANISOU 1480 CG PHE 212 17.010 8.950 64.912 1.000 23.33

ANISOU 1481 CD1 PHE 212 16.369 8.377 65.990 1.000 23.33

ANISOU 1481 CD1 PHE 212 2545 3115 3206 -382 -350 -5 ANISOU 1472 CB ALA 211 2957 4372 3906 834 -96 6 9 484 178 741 -30 -66 930 398 -128 3 7 4 284 -565 3 1 7 133 -640 6 8 -391 -406 2 2 2 293 -197 - 184 -376 -282 -558 ANISOU 1481 CD1 PHE 212 2545 3115 3206 -382 -350 - ATOM 1482 CD2 PHE 212 17.029 8.302 63.687 1.000 25.83 -382 -350 - 508 ANISOU 1482 CD2 PHE 212 2554 3962 3299 -622 -217 - ATOM 1483 CE1 PHE 212 15.730 7.149 65.872 1.000 28.13 -622 -217 -787ATOM 1483 CE1 PHE 212 15.730 7.149 65.872 1.000 28.13
ANISOU 1483 CE1 PHE 212 3784 3544 3362 -1119 96 - 97
ATOM 1484 CE2 PHE 212 16.419 7.072 63.569 1.000 23.04
ANISOU 1484 CE2 PHE 212 2504 2960 3289 382 -232 - 5
ATOM 1485 CZ PHE 212 15.781 6.486 64.651 1.000 27.88
ANISOU 1485 CZ PHE 212 3658 3977 2957 -1072 -501 - 7
ATOM 1486 N THR 213 19.076 12.936 63.578 1.000 18.30
ANISOU 1486 N THR 213 2690 2083 2181 149 -583 - 9
ATOM 1487 CA THR 213 19.566 14.310 63.681 1.000 17.99
ANISOU 1487 CA THR 213 1976 2139 2721 230 -686 - 2
ATOM 1488 CB THR 213 1976 2139 2721 230 -686 - 2
ATOM 1488 CB THR 213 1798 2280 3683 140 -119 - 4
ATOM 1489 OG1 THR 213 21.638 13.695 62.629 1.000 25.33
ANISOU 1489 OG1 THR 213 2571 3378 3676 925 71 5 2 8
ATOM 1490 CG2 THR 213 21.087 15.985 62.485 1.000 21.11
ANISOU 1490 CG2 THR 213 1935 2667 3420 -310 -289 - 7 -1119 96 - 973 -232 - 558-1072 -501 -760-583 - 93 -686 - 287 -119 - 423 71 5 2 8 ANISOU 1490 CG2 THR 213 1935 2667 3420 -310 -289 -747THR 213 18.391 15.277 63.641 1.000 15.53 ATOM 1491 C THR 213 1732 ANISOU 1491 C 2135 2032 111 -557 - 167 THR 213 17.533 15.195 62.761 1.000 16.11 ATOM 1492 0 THR 213 1742 ANISOU 1492 O 2197 -327 -669 5 6 2180 1493 N ASP 214 18.362 16.199 64.590 1.000 15.60 ASP 214 2025 ANISOU 1493 N 1857 2046 64 - 405 2 1494 CA ASP 214 17.380 17.256 64.672 1.000 15.59 ATOM ANISOU 1494 CA ASP 214 2130 1722 2072 2 -1010 - 242 ATOM 1495 CB ASP 214 17.744 18.200 65.822 1.000 17.13

- 139 -ANISOU 1495 CB ASP 214 2528 1893 2086 -226 -1022 -247ATOM 1496 CG ASP 214 17.612 17.672 67.219 1.000 20.21 ANISOU 1496 CG ASP 214 3138 2495 2045 -451 -1276 -451 -1276 -148 1497 OD1 ASP 214 17.079 16.571 67.460 1.000 20.87 ANISOU 1497 OD1 ASP 214 2778 2632 2518 -247 -505 1 5 1 ATOM 1498 OD2 ASP 214 18.076 18.401 68.127 1.000 28.05 ANISOU 1498 OD2 ASP 214 5110 3118 2429 -257 -1997 -1997 -619 ASP 214 17.314 18.146 63.441 1.000 15.14 1499 C ANISOU 1499 C ASP 214 2029 1822 1901 182 -574 - 319 ATOM 1500 0 ASP 214 18.349 18.552 62.897 1.000 17.63 ANISOU 1500 O ASP 214 1956 2032 2710 -214 -810 - 151501 N LEU 215 16.105 18.493 63.027 1.000 14.69 ATOM ANISOU 1501 N LEU 215 1936 1758 1887 38 - 334 242 ATOM 1502 CA LEU 215 15.915 19.504 61.979 1.000 13.35

ANISOU 1502 CA LEU 215 1820 1753 1498 89 -22 5 9

ATOM 1503 CB LEU 215 15.352 18.819 60.734 1.000 14.24

ANISOU 1503 CB LEU 215 1735 2167 1506 -98 75 - 3

ATOM 1504 CG LEU 215 16.291 17.813 60.056 1.000 16.39

ANISOU 1504 CG LEU 215 2031 2285 1911 -340 320 - 424

ATOM 1505 CD1 LEU 215 15.517 16.999 59.031 1.000 22.61

ANISOU 1505 CD1 LEU 215 3139 2024 3427 -10 -801 -877

ATOM 1506 CD2 LEU 215 17.482 18.543 59.434 1.000 26.93

ANISOU 1506 CD2 LEU 215 1998 5409 2827 -1083 909 -542

ATOM 1507 C LEU 215 15.002 20.622 62.500 1.000 14.65

ANISOU 1507 C LEU 215 1770 1607 2190 86 -165 -95

ATOM 1508 O LEU 215 1748 2165 3476 116 -303 -203

ATOM 1509 N PRO 216 15.552 21.523 63.314 1.000 15.99

ANISOU 1509 N PRO 216 2390 1970 1715 -164 21 -175

ATOM 1510 CD PRO 216 16.955 21.601 63.757 1.000 19.37 1502 CA LEU 215 15.915 19.504 61.979 1.000 13.35 ATOM ANISOU 1507 C ATOM ATOM 1510 CD PRO 216 2390 1970 1715 -164 21 -175
ANISOU 1510 CD PRO 216 2900 2306 2155 -83 -790 F -83 -790 - 548 1511 CA PRO 216 14.760 22.620 63.846 1.000 18.68 ATOM ANISOU 1511 CA PRO 216 3104 2017 1976 12 - 74 - 420 ATOM 1512 CB PRO 216 15.649 23.227 64.949 1.000 18.63 ANISOU 1512 CB PRO 216 3592 1517 1971 -120 -421 9 1513 CG PRO 216 17.030 22.847 64.581 1.000 22.35 ATOM ANISOU 1513 CG PRO 216 3401 2426 2666 -419 -427 - 783 ATOM 1514 C PRO 216 14.461 23.700 62.819 1.000 18.50 ANISOU 1514 C ANISOU 1514 C PRO 216 2921 2083 2026 58-465 -47
ATOM 1515 O PRO 216 15.024 23.854 61.731 1.000 19.82
ANISOU 1515 O PRO 216 2752 2453 2325 -32 -375 1
ATOM 1516 N TYR 217 13.487 24.536 63.194 1.000 20.05
ANISOU 1516 N TYR 217 3213 1981 2422 90 -482 -71
ATOM 1517 CA TYR 217 13.178 25.662 62.308 1.000 22.97
ANISOU 1517 CA TYR 217 13.178 25.662 62.308 1.000 22.97
ANISOU 1518 C TYR 217 14.347 26.647 62.283 1.000 23.92
ANISOU 1518 C TYR 217 4139 2131 2819 -337 -1776 ATOM 1519 O TYR 217 4391 2819 -337 -1776 ATOM 1519 O TYR 217 4321 3440 3812 -1118 -2477 7
ANISOU 1520 CB TYR 217 11.891 26.314 62.768 1.000 32.68
ANISOU 1520 CB TYR 217 3958 3294 5164 1148 -874 -7
ANISOU 1521 CG TYR 217 6829 4326 5854 895 38 -18 PRO 216 2921 2083 2026 58 - 465 - 473 -375 1 9 90 - 482 - 718-1467 -313 -337 -1776 -165 -1118 -2477 7 2 8 1148 -874 - 783 ANISOU 1521 CG TYR 217 6829 4326 5854 895 38 - 1870 1522 CD1 TYR 217 11.853 28.763 63.285 1.000 54.26 ANISOU 1522 CD1 TYR 217 10311 -323 132 -1945 3688 6615 1523 CD2 TYR 217 12.428 27.243 65.043 1.000 57.77 ANISOU 1523 CD2 TYR 217 10635 5155 6158 -1027 -1446 -1931 1524 CE1 TYR 217 12.011 29.816 64.174 1.000 60.33 ANISOU 1524 CE1 TYR 217 11807 4345 6772 -1101 -132 -2259 1525 CE2 TYR 217 12.585 28.296 65.926 1.000 64.51 ANISOU 1525 CE2 TYR 217 12481 5199 6832 -1936 -1520 -2074

	- 140 -	
ATOM 1526 CZ TYR		65.481 1.000 64.11
ANISOU 1526 CZ TYR	217 12047 5183	7129 -1460 -817 -2160
ATOM 1527 OH TYR		66.358 1.000 63.69
ANISOU 1527 OH TYR		7153 -1832 -1191 -2064
ATOM 1528 N ARG ANISOU 1528 N ARG		61.188 1.000 24.08
ATOM 1529 CA ARG		3055 507 -1471 -145
ANISOU 1529 CA ARG		60.948 1.000 30.71 3245 -504 -1565 382
ATOM 1530 CB ARG		59.840 1.000 35.08
ANISOU 1530 CB ARG	218 5969 2797	4562 -1397 -779 - 348
ATOM 1531 CG ARG		60.073 1.000 35.77
ANISOU 1531 CG ARG ATOM 1532 CD ARG		4497 -1107 -733 - 773
ANISOU 1532 CD ARG		60.626 1.000 34.46 4152 -1242 -244 -619
ATOM 1533 NE ARG		4152 -1242 -244 - 619 59.709 1.000 29.51
ANISOU 1533 NE ARG	218 4707 2579	3926 78 81 - 62 9
ATOM 1534 CZ ARG		58.830 1.000 33.18
ANISOU 1534 CZ ARG ATOM 1535 NH1 ARG		4170 60 452 - 1075
ATOM 1535 NH1 ARG ANISOU 1535 NH1 ARG		58.709 1.000 27.44
ATOM 1536 NH2 ARG		3341 -503 -373 -1585 58.077 1.000 22.96
ANISOU 1536 NH2 ARG	218 2327 3579	2817 233 -1117 - 872
ATOM 1537 C ARG	218 14.513 29.655	60.464 1.000 31.05
ANISOU 1537 C ARG ATOM 1538 O ARG	· · · · · · · · · · · · · · · · · · ·	2496 -448 -1823 197
ATOM 1538 O ARG ANISOU 1538 O ARG		59.295 1.000 40.40 3235 531 -3168 -627
ATOM 1539 N PRO		3235 531 -3168 -627 61.157 1.000 30.01
ANISOU 1539 N PRO	219 6290 2559	2555 -499 -1839 - 284
ATOM 1540 CD PRO		62.543 1.000 36.79
ANISOU 1540 CD PRO ATOM 1541 CA PRO		2954 -1848 -2548 - 374
ANISOU 1541 CA PRO		60.549 1.000 26.34 3025 -573 -988 -340
ATOM 1542 CB PRO		61.563 1.000 32.44
ANISOU 1542 CB PRO	219 5361 2891	4073 -691 -417 - 989
ATOM 1543 CG PRO		62.825 1.000 38.75
ANISOU 1543 CG PRO ATOM 1544 C PRO		3344 -1981 -958 -1235
ANISOU 1544 C PRO		59.220 1.000 23.64 3443 -161 -1028 1 0 9
ATOM 1545 O PRO		58.412 1.000 30.61
ANISOU 1545 O PRO	219 4358 2934	4339 -347 -1712 8 7 6
ATOM 1546 N ASP ANISOU 1546 N ASP		58.906 1.000 25.98
ATOM 1547 CA ASP	220 3611 1756 220 15.847 32.660	4506 -389 -644 -815
ANISOU 1547 CA ASP		57.705 1.000 27.96 5071 -364 30 -824
ATOM 1548 CB ASP	220 17.212 33.238	58.155 1.000 29.61
ANISOU 1548 CB ASP	220 3549 3142	4558 -176 -326 1 7 6
ATOM 1549 CG ASP ANISOU 1549 CG ASP		58.780 1.000 32.09
ATOM 1550 OD1 ASP		4961 625 978 615 59.719 1.000 26.12
ANISOU 1550 OD1 ASP	220 3013 3522	3390 -158 -289 - 9 7
ATOM 1551 OD2 ASP	220 19.241 32.088	58.281 1.000 29.09
ANISOU 1551 OD2 ASP		3581 304 677 - 712
ATOM 1552 C ASP ANISOU 1552 C ASP		56.525 1.000 25.26
ATOM 1553 O ASP		5800 354 1110 - 822 55.515 1.000 28.28
ANISOU 1553 O ASP		4994 -855 298 -434
ATOM 1554 N ALA	221 15.500 30.510	56.631 1.000 21.58
ANISOU 1554 N ALA ATOM 1555 CA ALA	· -	3681 -288 178 -651
ATOM 1555 CA ALA ANISOU 1555 CA ALA		55.658 1.000 19.81 3090 -342 -224 - 315
ATOM 1556 CB ALA	221 2386 1432	

- 141 -ANISOU 1556 CB ALA 221 2267 1497 3647 -648 45 -74
ATOM 1557 C ALA 221 14.718 28.469 55.489 1.000 17.71
ANISOU 1557 C ALA 221 2304 1912 2512 -251 -75 -3
ATOM 1558 O ALA 221 13.866 28.356 56.380 1.000 20.97
ANISOU 1558 O ALA 221 3596 2029 2344 -503 406 -2
ATOM 1559 N VAL 222 14.728 27.756 54.378 1.000 14.22 -648 45 - 746 -251 -75 -309 -503 406 -284 VAL 222 15.720 2262 -76 -92 -11 1560 CA VAL 222 13.823 26.617 54.160 1.000 14.89 ATOM ANISOU 1560 CA VAL 222 1326 1608 2723 98 - 216 - 205 1561 CB VAL 222 1320 1006 2723 98 -216 -20 1561 CB VAL 222 13.079 26.779 52.830 1.000 17.28 J 1561 CB VAL 222 1680 1754 3133 90 -657 -14 ANISOU 1561 CB VAL 222 1680 1754 3133 90 -657 -144 1562 CG1 VAL 222 13.995 26.685 51.620 1.000 19.17 ANISOU 1562 CG1 VAL 222 1974 2625 2686 -446 -775 1 5 0 1563 CG2 VAL 222 11.996 25.747 52.641 1.000 17.36 ATOM ANISOU 1563 CG2 VAL 222 2185 1879 2533 -254 -362 - 385 VAL 222 14.653 25.339 54.263 1.000 12.66 ATOM 1564 C ANISOU 1564 C 1564 VAL 222 1136 2112 -50 -225 - 378 VAL 222 15.828 25.320 53.893 1.000 13.12 ATOM 1565 0 ANISOU 1565 O VAL 222 1280 1825 1881 104 -13 -199 MOTA1566 N LEU 223 14.049 24.267 54.775 1.000 12.98 ANISOU 1566 N LEU 223 1123 1538 2270 -163 -370 -417 ATOM 1567 CA LEU 223 14.681 22.952 54.749 1.000 10.70 ANISOU 1567 CA LEU 223 891 1704 1472 -26 -98 - 7 ATOM 1568 CB LEU 223 14.276 22.130 55.961 1.000 13.02 ANISOU 1568 CB LEU 223 1387 1968 1593 -419 289 ATOM 1569 CG LEU 223 14.739 20.683 56.106 1.000 17.41 -419 289 -108
 223
 2434
 2132
 2050
 -290
 -476
 56

 223
 16.247
 20.614
 56.204
 1.000
 17.20

 223
 2576
 1518
 2441
 26-989
 -24

 223
 13.983
 20.076
 57.282
 1.000
 33.63

 223
 3981
 4721
 4077
 -341
 134
 29

 223
 14.362
 22.211
 53.456
 1.000
 10.02
 20
 ANISOU 1569 CG LEU -290 -476 5 6 6 1570 CD1 LEU ATOM ANISOU 1570 CD1 LEU 26 - 989 - 249 ATOM 1571 CD2 LEU ANISOU 1571 CD2 LEU -341 134 2949 ATOM 1572 C LEU ANISOU 1572 C LEU 223 1000 1265 1543 58 - 319 8 8 223 13.206 22.160 53.088 1.000 12.86 ATOM 1573 0 LEU ANISOU 1573 O LEU 223 949 1945 1992 -97 -174 -372 1574 N ATOM VAL 224 15.406 21.675 52.798 1.000 10.55 ANISOU 1574 N VAL 224 978 1070 1962 -76 -418 -382 MOTA 1575 CA VAL 224 15.227 20.932 51.553 1.000 11.98 ANISOU 1575 CA VAL 224 1376 1288 1887 -249 -278 - 372 ATOM 1576 CB VAL 224 16.095 21.461 50.391 1.000 11.23
ANISOU 1576 CB VAL 224 901 1541 1824 -279 -622 -999
ATOM 1577 CG1 VAL 224 15.833 20.690 49.102 1.000 13.16
ANISOU 1577 CG1 VAL 224 1899 1485 1615 -462 -516 8 4
ATOM 1578 CG2 VAL 224 15.837 22.941 50.156 1.000 13.86
ANISOU 1578 CG2 VAL 224 1480 1520 2266 -135 -354 -6
ATOM 1579 C VAL 224 15.539 19.450 51.786 1.000 10.87
ANISOU 1579 C VAL 224 953 1275 1901 -13 342 -484
ATOM 1580 O VAL 224 16.646 19.148 52.201 1.000 12.57
ANISOU 1580 O VAL 224 1283 1363 2132 -175 -154 -2
ATOM 1581 N PHE 225 14.585 18.553 51.533 1.000 11.86
ANISOU 1581 N PHE 225 14.585 18.553 51.533 1.000 11.86
ANISOU 1582 CA PHE 225 14.811 17.130 51.412 1.000 11.38
ANISOU 1582 CA PHE 225 1260 1157 1909 -22 -67 -5
ATOM 1583 CB PHE 225 13.707 16.280 52.044 1.000 11.34 ATOM 1576 CB VAL 224 16.095 21.461 50.391 1.000 11.23 -462 -51684 2266 -135 -354 - 64 -175 -154 - 274 -303 **-** 61 -67 -56 1583 CB PHE 225 13.707 16.280 52.044 1.000 11.34 ANISOU 1583 CB PHE 225 1117 1176 2015 205 1583 CB PHE 225 1117 1176 2015 205 -213 3 1584 CG PHE 225 13.654 16.172 53.544 1.000 11.38 ANISOU 1584 CG PHE 225 964 1369 1991 -251 -333 181 1585 CD1 PHE 225 14.685 15.653 54.291 1.000 15.28 ANISOU 1585 CD1 PHE 225 1771 1777 2256 -98 -853 2 9 8 MOTA 1586 CD2 PHE 225 12.532 16.576 54.254 1.000 17.91 ANISOU 1586 CD2 PHE 225 1904 2748 2153 341 106 0

- 142 -1587 CE1 PHE 225 14.619 15.535 55.661 1.000 17.46 ATOM ANISOU 1587 CE1 PHE 225 2449 1862 2321 -249 -795 6 6 6 1588 CE2 PHE 225 12.447 16.474 55.612 1.000 19.35 ANISOU 1588 CE2 PHE 225 2563 2678 2111 121 129 - 11 1589 CZ PHE 225 13.499 15.945 56.341 1.000 18.20 ATOM ANISOU 1589 CZ PHE 225 2952 1641 2324 -501 -470 3 6 ATOM 1590 C PHE 225 14.907 16.774 49.927 1.000 12.03 ANISOU 1590 C PHE 225 1480 1285 1804 130 -201 4 2 ATOM 1591 O PHE 225 14.019 17.160 49.163 1.000 12.77 ANISOU 1591 O PHE 225 1473 1466 1912 341 -118 3 8 ATOM 1592 N CYS 226 15.940 16.032 49.521 1.000 9.62 ANISOU 1592 N CYS 226 954 1403 1296 -204 -407 2 9 ATOM 1593 CA CYS 226 15.917 15.400 48.197 1.000 10.80 ANISOU 1593 CA CYS 226 1432 1204 1468 -258 -310 - 5 9 ATOM 1594 CB CYS 226 17.337 15.029 47.744 1.000 12.02 ANISOU 1594 CB CYS 226 1539 1362 1666 -357 16 -125 ATOM 1595 SG CYS 226 1627 1400 2192 -341 18 13 9 ATOM 1596 C CYS 226 1627 1400 2192 -341 18 13 9 ATOM 1596 C CYS 226 14.998 14.178 48.256 1.000 9.86 ANISOU 1596 C CYS 226 1190 1061 1495 -20 -293 - 16 ATOM 1597 O CYS 226 15.015 13.431 49.252 1.000 11.17 1590 C PHE 225 14.907 16.774 49.927 1.000 12.03 ATOM ANISOU 1596 C CYS 226 1190 1061 1495 -20 -293 - 16 ATOM 1597 O CYS 226 15.015 13.431 49.252 1.000 11.17 ANISOU 1597 O CYS 226 1181 1280 1781 -129 -435 2 7 2 ATOM 1598 N GLY 227 14.217 13.963 47.205 1.000 10.17 J 1598 N GLY 227 1428 1010 1427 -258 -271 - 35 1599 CA GLY 227 13.370 12.806 47.053 1.000 9.73 ANISOU 1598 N ATOM ANISOU 1599 CA GLY 227 1231 860 1604 -178 -74 - 37 ATOM 1600 C GLY 227 13.3908 11.769 46.074 1.000 9.48 ANISOU 1600 C GLY 227 1438 717 1445 16 -35 169 ATOM 1601 O GLY 227 13.21 1137 1290 -104 -179 7 ATOM 1602 N ALA 228 13.217 10.631 45.971 1.000 9.17 ANISOU 1602 N ALA 228 13.650 9.529 45.108 1.000 9.41 ANISOU 1603 CA ALA 228 1315 887 1371 9 -74 - 52 ATOM 1604 CB ALA 228 13.712 8.296 45.256 1.000 10.50 ANISOU 1605 C ALA 228 13.712 9.918 43.637 1.000 9.25 ANISOU 1605 C ALA 228 13.712 9.918 43.637 1.000 9.25 ANISOU 1606 O ALA 228 13.712 9.918 43.637 1.000 9.25 ANISOU 1606 O ALA 228 13.712 9.918 43.637 1.000 9.25 ANISOU 1606 O ALA 228 13.712 9.918 43.637 1.000 9.48 ANISOU 1606 O ALA 228 1171 1026 1405 -88 -50 9 ATOM 1607 N ILE 229 12.970 10.907 43.143 1.000 10.30 ANISOU 1608 CA ILE 229 13.074 11.311 41.727 1.000 10.87 ATOM 1608 CA ILE 229 13.074 11.311 41.727 1.000 10.87 ANISOU 1608 CA ILE 229 13.074 11.311 41.727 1.000 10.87 ANISOU 1608 CA ILE 229 1197 1446 1487 -2 -159 251 ATOM 1609 CB ILE 229 11.802 12.078 41.295 1.000 11.52 ANISOU 1599 CA GLY 227 1231 860 1604 -178 -74 - 37 -104 -179 7 8 -88 -50 9 0 ATOM 1609 CB ILE 229 11.802 12.078 41.295 1.000 10.87 ANISOU 1609 CB ILE 229 1257 1473 1647 34 -57 3 6 2 ATOM 1610 CG2 ILE 229 11.007 -2 -159 2 5 1 ATOM 1610 CG2 ILE 229 11.997 12.852 39.999 1.000 11.30 ANISOU 1610 CG2 ILE 229 1655 1211 1426 83 -189 15 83 - 189 156 ATOM 1611 CG1 ILE 229 10.575 11.131 41.237 1.000 14.39 ANISOU 1611 CG1 ILE 229 1031 2034 2402 -40 210 311 ATOM 1612 CD1 ILE 229 10.676 10.093 40.138 1.000 19.20 ANISOU 1612 CD1 ILE 229 2085 1723 3489 -610 93 -13 ATOM 1613 C ILE 229 14.389 12.034 41.477 1.000 10.38 -610 93 - 138 ATOM 1613 C ILE 229 14.389 12.034 41.477 1.000 10.38

ANISOU 1613 C ILE 229 1293 1405 1247 -62 -169 3 2 2

ATOM 1614 O ILE 229 14.952 11.947 40.369 1.000 11.66

ANISOU 1614 O ILE 229 1805 1257 1368 -13 145 3 2 8

ATOM 1615 N ALA 230 14.965 12.692 42.490 1.000 10.66

ANISOU 1615 N ALA 230 1476 1274 1300 -104 -151 3 5 6

ATOM 1616 CA ALA 230 16.312 13.259 42.338 1.000 11.21

ANISOU 1616 CA ALA 230 1473 975 1813 -57 -308 9 0

ATOM 1617 CB ALA 230 16.681 14.148 43.509 1.000 10.58

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						- 143 -		
ANISOU	1617	СB	ALA	230	1350	1295	1375	62 - 106 126
ATOM	1618		ALA		17.336			
						12.136		1.000 11.28
ANISOU			ALA		1640	1037	1610	1 55 2 4 2
\mathtt{ATOM}	1619	0	ALA	230	18.220	12.185	41.273	1.000 11.29
ANISOU			ALA		1510			
						1240	1539	-189 -40 288
\mathtt{ATOM}	1620		THR	231	17.173	11.097	42.946	1.000 10.55
ANISOU	1620	N	THR		1328	894 17		52 -70 2 1 4
ATOM	1621							
			THR		18.064	9.939	42.819	1.000 11.98
ANISOU	1621	CA	THR	231	1929	1018	1605	0 -164 159
ATOM	1622	CB	THR	231	17.717	8.865	43.878	1.000 10.76
ANISOU								
			THR		1381	1070	1636	-86 -453 2 4 6
ATOM	1623	OG1	THR	231	17.658	9.437	45.198	1.000 11.82
ANISOU	1623	OG1	THR		1615	1236	1641	
ATOM	1624					7.550		
	1024	CG2	Ink		18.765	7.752	43.880	1.000 12.57
ANISOU			THR	231	1621	1314	1840	160 -89 351
ATOM	1625	С	THR	231	17.958	9.352	41.415	1.000 12.52
ANISOU			THR		1632			
						1500	1624	-145 42 1 1
ATOM	1626		\mathtt{THR}	231	18.939	9.050	40.732	1.000 12.15
ANISOU	1626	0	THR	231	1636	1233	1747	-17 86 2 2 4
ATOM	1627		LEU	333	16.717			
				272	10.717	9.154	40.959	1.000 11.14
ANISOU			LEU		1608	1005	1620	90 -68 1 4 1
ATOM	1628	CA	LEU	232	16.446	8.522	39.675	1.000 12.47
ANISOU	1628	CA	LEU		1880	1203		
							1657	109 -169 4 5
ATOM	1629		LEU		14.950	8.214	39.552	1.000 12.81
ANISOU	1629	CB	LEU	232	1989	1225	1654	-78 -209 1 9
ATOM	1630	CG	LEU		14.452	7.464	38.314	1.000 14.85
ANISOU								
			LEU		2171	1753	1719	-5 -410 - 96
\mathtt{ATOM}	1631			232	15.020	6.055	38.240	1.000 16.78
ANISOU	1631	CD1	LEU	232	2693	1749		72 -431 -487
ATOM	1632				12.914			
	1032	CDZ	TEO			7.411	38.291	1.000 15.70
ANISOU			LEU		2180	1866	1920	-278 -589 4 9 4
\mathtt{ATOM}	1633	C	LEU	232	16.964	9.354	38.511	1.000 11.58
ANISOU			LEU		1452			
						1390	1559	309 -301 1 3 6
ATOM	1634		LEU		17.752	8.837	37.686	1.000 13.45
ANISOU	1634	0	LEU	232	1808	1436	1867	320 -17 3 0
ATOM	1635	N	VAL	233	16.565	10.617	38.414	1.000 10.95
ANISOU								
			VAL		1428	1210	1522	-14 -210 0
ATOM	1636		VAL	233	16.948	11.421	37.242	1.000 11.70
ANISOU	1636	CA	VAL		1703	1345	1397	975 1 3
ATOM	1637							
			VAL		16.156	12.743	37.215	1.000 11.14
ANISOU			VAL		1672	1272	1287	-26 276 7 3
\mathtt{ATOM}	1638	CG1	VAL	233	16.661	13.774	38.249	1.000 13.34
ANISOU							1672	-205 653 -368
					1024			
ATOM	1639	CGZ	VAL		16.106	13.412	35.827	1.000 14.66
ANISOU	1639	CG2	VAL	233	1992	1873	1704	-4 -45 5 8 6
ATOM	1640	C	VAL	233	18.459	11.586	37.132	1.000 13.41
ANISOU								
			VAL		1712	1573	1811	91 151 1 2 5
\mathtt{ATOM}	1641		VAL	233	19.012	11.627	36.021	1.000 13.45
ANISOU	1641	0	VAL		1844	1402	1866	46 192 4 3 8
ATOM	1642		THR					
					19.188	11.665	38.250	1.000 13.13
ANISOU			THR	234	1457	1639	1893	-139 223 126
ATOM	1643	CA	THR		20.613	11.930	38.244	1.000 13.00
ANISOU	1643	40	THR		1483	1600		
ATOM							1855	-188 428 1 4 3
	1644	CB	THR		21.069	12.726	39.465	1.000 12.46
ANISOU			\mathtt{THR}	234	1300	1632	1803	-32 200 251
ATOM	1645	0G1			20.825	11.941	40.639	1.000 13.71
ANISOU								
					1660	1662	1888	192 202 291
ATOM	1646	CG2	\mathtt{THR}	234	20.301	14.027	39.643	1.000 11.37
ANISOU	1646	CG2	THR		1097	1565	1657	-153 -87 169
ATOM	1647		THR		21.424			
ANISOU				774	41.444	10.643	38.178	1.000 14.44
WINT 200	T04/		THR	∠ 3 4	1550	1823	2114	6 -73 - 53

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				- 1-4-4 -		
ATOM 1648 C		234	22.659	10.710	38.233	1.000 15.81
ANISOU 1648 C	THR	234	1546	2169	2293	61 27 2 1 7
ATOM 1649 N	W GLY		20.767	9.477	38.070	1.000 14.76
ANISOU 1649 N						
			1776	1576	2254	77 81 4 1 0
ATOM 1650 C			21.530	8.249	37.994	1.000 16.69
ANISOU 1650 C		235	2053	1803	2486	304 35 1 8 9
ATOM 1651 C	GLY	235	22.243	7.862	39.275	1.000 16.83
ANISOU 1651			1854			
_				2031	2512	765 244 193
			23.305	7.237	39.194	1.000 19.67
ANISOU 1652 C			2074	2172	3225	1035 383 372
ATOM 1653 N	J GLY	236	21.665	8.227	40.425	1.000 14.46
ANISOU 1653 N	W GLY		1732	1327	2433	
ATOM 1654 C			22.187	7.768		
ANISOU 1654 C					41.692	1.000 15.73
			2060	1381	2536	41 186 3 1 2
ATOM 1655 C			23.166	8.691	42.388	1.000 14.76
ANISOU 1655 C	C GLY	236	1931	1332	2346	252 73 2 8 8
ATOM 1656 C	GLY		23.778	8.244	43.373	1.000 18.32
ANISOU 1656 C			1983	2197		
ATOM 1657 N					2782	106 -105 8 4 4
			23.318	9.938	41.953	1.000 13.99
ANISOU 1657 N			1831	1349	2137	158 165 170
ATOM 1658 C		237	24.209	10.956	42.485	1.000 13.13
ANISOU 1658 C	CA GLN	237	1474	1304	2210	367 -31 276
ATOM 1659 C			24.629	11.948	41.383	1.000 13.38
ANISOU 1659 C			1367			
ATOM 1660 C				1566	2151	99 72 1 5 9
			25.390	11.335	40.219	1.000 14.74
ANISOU 1660 C			1404	1529	2666	518 410 333
ATOM 1661 C		237	25.816	12.428	39.257	1.000 17.22
ANISOU 1661 C	CD GLN	237	2039	2018	2486	-64 426 360
ATOM 1662 C	E1 GLN		26.754	13.208	39.522	1.000 20.60
ANISOU 1662 C	OF1 CLM		1566			
	NE2 GLN			2334	3928	-10 -29 965
			25.116	12.470	38.127	1.000 17.47
ANISOU 1663 N			2014	2093	2533	208 438 408
ATOM 1664 C	GLN	237	23.627	11.739	43.663	1.000 12.90
ANISOU 1664 C	GLN	237	1474	1324	2104	72 -10 2 5 5
ATOM 1665 C		237	24.332	12.549	44.282	1.000 15.90
ANISOU 1665 C			1739			
ATOM 1666 N				1888	2413	-291 74 - 84
			22.365	11.481	44.013	
ANISOU 1666 N			1372		76 21:	
ATOM 1667 C		238	21.664	12.182	45.082	1.000 11.91
ANISOU 1667 C	CA VAL	238	1169	1436	1920	-121 -276 - 19
ATOM 1668 C	CB VAL		20.622	13.158	44.510	1.000 12.00
ANISOU 1668 C	B VAL		1024			
	G1 VAL			1179	2357	-6 199 - 3 1
ANTCOU 1009 C	GI VAL		19.978	13.999		1.000 13.07
ANISOU 1669 C	GI VAL		1530	1668		63 -232 - 222
ATOM 1670 C	CG2 VAL	238	21.207	14.088	43.463	1.000 14.00
ANISOU 1670 C	G2 VAL	238	1795	1470	2053	-40 -2 1 8 1
ATOM 1671 C	VAL		20.990	11.156	46.000	
ANISOU 1671	VAL		1707	1415		
ATOM 1672 C					2054	-103 -40 - 22
			20.252			1.000 12.64
ANISOU 1672			1702	977 21:	23 60	-318 257
ATOM 1673 N			21.247	11.246	47.300	1.000 11.99
ANISOU 1673 N		239	1075	1404	2076	127 -101 7 4
ATOM 1674 C	CA LYS		20.568	10.444	48.322	1.000 12.77
ANISOU 1674 C	CA LYS		1224	1541	2088	-12 -124 8 6
ATOM 1675 C			21.382			
ANISOU 1675 C				10.463	49.622	1.000 12.23
			1333	1155	2158	183 -234 - 28
ATOM 1676 C			20.953	9.626	50.793	1.000 13.85
ANISOU 1676 C			1643	1689	1931	187 -52 - 8 9
ATOM 1677 C		239	21.927	9.579	51.957	1.000 20.13
ANISOU 1677 (CD LYS		2893	1795	2961	
ATOM 1678 (21.364	8.745		1.000 24.73
·				J . / T J	55.030	1.000 6 4 . / J

		145	
ATOM 1679 NZ ANISOU 1679 NZ ATOM 1680 C ANISOU 1681 O ANISOU 1682 N ANISOU 1683 CA ANISOU 1683 CA ANISOU 1683 CA ANISOU 1684 CB ANISOU 1685 C ANISOU 1685 C ANISOU 1686 O ANISOU 1687 N ANISOU 1687 N ANISOU 1688 CD ATOM 1689 CA ANISOU 1689 CA ANISOU 1689 CA ANISOU 1689 CA ANISOU 1690 CB ANISOU 1691 CG ANISOU 1691 CG ANISOU 1692 C ANISOU 1692 C ANISOU 1693 O ANISOU 1693 O ANISOU 1693 O ANISOU 1694 N ANISOU 1694 N ANISOU 1695 CA ANISOU 1695 CA ANISOU 1695 CA ANISOU 1696 CB ANISOU 1697 CG ANISOU 1697 CG ANISOU 1699 NE ANISOU 1699 CB ANISOU 1699 NE ANISOU 1700 CZ ANISOU 1701 NH1 ANISOU 1701 NH1 ANISOU 1702 NH2 ANISOU 1703 C ANISOU 1703 C ANISOU 1704 O ANISOU 1704 O	ARG 242 3225 ARG 242 16.107 ARG 242 3198 ARG 242 15.285 ARG 242 4097 ARG 242 17.416 ARG 242 3402 ARG 242 14.477 ARG 242 1571 ARG 242 15.469 ARG 242 1708	4315 2293 10.949 48.661 1332 1866 12.191 48.708 1294 1749 10.047 48.863 1266 1534 10.368 49.354 1057 1531 9.782 48.466 2378 1543 9.881 50.807 1249 1611 8.664 51.059 1242 1568 10.783 51.782 1041 1466 12.237 51.654 12.04 1618 10.340 53.166 1447 1499 11.545 53.891 1837 1701 12.724 53.069 1446 1709 10.072 53.861 1610 1665 10.829 53.655 1582 1723 9.033 54.711 1407 1664 8.804 55.576 1417 1380 7.405 <td>1.000 32.28 1610 -930 - 304 1.000 11.59 -35 -82 6 4 1.000 12.32 -2 -25 2 3 6 1.000 10.65 -52 -185 - 8 8 1.000 10.21 -195 -37 -109 1.000 13.46 -232 20 -403 1.000 10.97 -127 -142 4 9 1.000 13.02 -243 28 - 7 1.000 11.13 160 -49 1 3 8 1.000 11.17 -180 -128 7 6 1.000 11.96 -172 -32 1 9 3 1.000 12.35 -531 -383 2 4 2 1.000 13.61 -596 -465 - 2 2 1.000 12.35 -175 -187 4 1 8 1.000 12.28 -232 -468 8 1 1.000 12.75 -170 76 2 5 0 1.000 10.76 -207 -281 2 1 1 1.000 15.02 -357 117 2 9 4 1.000 17.85 9 -560 2 5 1 1.000 19.42 506 503 1 1 6 1.000 20.71 938 638 2 1 2 1.000 23.22 307 -544 5 8 9 1.000 24.46 307 387 1 9 5 1.000 25.41 819 -267 4 0 3 1.000 11.95 -248 -214 1 0 7 1.000 13.65 -322 -401 - 3 8</td>	1.000 32.28 1610 -930 - 304 1.000 11.59 -35 -82 6 4 1.000 12.32 -2 -25 2 3 6 1.000 10.65 -52 -185 - 8 8 1.000 10.21 -195 -37 -109 1.000 13.46 -232 20 -403 1.000 10.97 -127 -142 4 9 1.000 13.02 -243 28 - 7 1.000 11.13 160 -49 1 3 8 1.000 11.17 -180 -128 7 6 1.000 11.96 -172 -32 1 9 3 1.000 12.35 -531 -383 2 4 2 1.000 13.61 -596 -465 - 2 2 1.000 12.35 -175 -187 4 1 8 1.000 12.28 -232 -468 8 1 1.000 12.75 -170 76 2 5 0 1.000 10.76 -207 -281 2 1 1 1.000 15.02 -357 117 2 9 4 1.000 17.85 9 -560 2 5 1 1.000 19.42 506 503 1 1 6 1.000 20.71 938 638 2 1 2 1.000 23.22 307 -544 5 8 9 1.000 24.46 307 387 1 9 5 1.000 25.41 819 -267 4 0 3 1.000 11.95 -248 -214 1 0 7 1.000 13.65 -322 -401 - 3 8
ANISOU 1702 NH2	ARG 242 3402	2332 3921	819 -267 4 0 3
ATOM 1703 C	ARG 242 14.477	9.834 56.704	1.000 11.95
ANISOU 1703 C	ARG 242 1571	1463 1506	-248 -214 1 0 7
ANISOU 1704 O	ARG 242 1708	1439 2040	-322 -401 - 38
ATOM 1705 N	HIS 243 13.252	10.085 57.118	1.000 11.60
ANISOU 1705 N	HIS 243 1657	1410 1342	-311 -206 5
ATOM 1706 CA	HIS 243 12.942	11.056 58.158	1.000 11.49
ANISOU 1706 CA	HIS 243 1855	1571 938 -3	06 -183 140
ATOM 1707 CB	HIS 243 12.968	12.462 57.546	1.000 11.22
ANISOU 1707 CB	HIS 243 1432	1379 1453	-231 -221 3 9
ATOM 1708 CG	HIS 243 12.133	12.694 56.341	
ANISOU 1708 CG	HIS 243 1937	1171 1378	

- 146 -ATOM 1709 CD2 HIS 243 10.885 13.236 56.181 1.000 11.15 ANISOU 1709 CD2 HIS 243 1990 1106 1142 35 -344 14: ATOM 1710 ND1 HIS 243 12.538 12.345 55.086 1.000 12.29 35 - 344 141 243 1670 ANISOU 1710 ND1 HIS 1606 1395 -394 -91 243 11.599 12.653 54.209 1.000 12.59 1711 CE1 HIS ATOM ANISOU 1711 CE1 HIS 243 1686 1740 1357 -522 -202 - 253 243 10.585 13.204 54.841 1.000 10.77 1712 NE2 HIS ATOM ANISOU 1712 NE2 HIS 243 1612 1307 1172 -616 -268 - 36 1713 C HIS 243 11.605 10.737 58.812 1.000 12.49 ATOM ANISOU 1713 C HIS 243 1869 1570 1308 -321 -53 7 3 1714 O HIS 243 10.807 9.949 58.271 1.000 12.26 ATOM ANISOU 1714 O HIS 243 1756 1404 1497 -188 -115 4 7 1715 N HIS 244 11.352 11.319 59.983 1.000 12.16 ANISOU 1715 N HIS 244 1464 1715 1442 -230 -112 - 32 1716 CA HIS 244 10.138 11.043 60.758 1.000 12.02 ANISOU 1716 CA HIS 244 1606 1809 1152 -599 -167 - 24 ATOM 1717 CB HIS 244 10.255 9.778 61.615 1.000 12.51 ANISOU 1717 CB HIS 244 1655 1763 1334 -19 101 -47 ATOM 1718 CG HIS 244 11.270 9.810 62.698 1.000 15.04

ANISOU 1718 CG HIS 244 2025 1733 1965 -178 -433 15 4

ATOM 1719 CD2 HIS 244 21.276 10.380 63.923 1.000 18.19

ANISOU 1719 CD2 HIS 244 2946 2339 1627 36 -732 297

ATOM 1720 ND1 HIS 244 12.504 9.203 62.662 1.000 19.30

ANISOU 1720 ND1 HIS 244 13.226 9.387 63.731 1.000 22.48

ATOM 1721 CE1 HIS 244 13.226 9.387 63.731 1.000 22.48

ANISOU 1721 CE1 HIS 244 13.226 9.387 63.731 1.000 22.38

ANISOU 1722 NE2 HIS 244 24.76 10.120 64.531 1.000 22.33

ANISOU 1722 NE2 HIS 244 12.476 10.120 64.531 1.000 22.33

ANISOU 1722 NE2 HIS 244 18.897 1673 1549 -362 254 67

ATOM 1724 O HIS 244 18.897 1673 1549 -362 254 67

ATOM 1725 N VAL 245 8.551 12.246 61.613 1.000 13.48

ANISOU 1725 N VAL 245 8.551 12.245 62.130 1.000 13.48

ANISOU 1725 N VAL 245 8.551 12.245 62.130 1.000 15.26

ANISOU 1726 CA VAL 245 8.090 13.352 62.970 1.000 15.26

ANISOU 1727 CB VAL 245 6.939 14.169 62.360 1.000 17.31

ANISOU 1727 CB VAL 245 6.939 14.169 62.360 1.000 17.33

ANISOU 1727 CB VAL 245 6.939 14.169 62.360 1.000 17.33

ANISOU 1727 CB VAL 245 6.951 15.334 63.286 1.000 17.33

ANISOU 1728 CGI VAL 245 2094 2473 2019 -80 340 -47

ATOM 1728 CGI VAL 245 7.252 14.713 60.966 1.000 25.25

ANISOU 1730 C VAL 245 8.090 2538 2550 -180 313 271

ATOM 1730 C VAL 245 1810 2174 3089 -15 451 254

ANISOU 1731 O VAL 245 1810 2174 3089 -15 451 254

ANISOU 1731 O VAL 245 1810 2174 3089 -15 451 254

ANISOU 1731 O VAL 245 1810 2174 3089 -15 451 254

ANISOU 1731 C VAL 245 1810 2174 3089 -15 451 254

ANISOU 1731 C A ALA 246 8.385 13.202 65.369 1.000 25.10

ANISOU 1733 CA ALA 246 8.381 3045 2327 -447 509 -79 74070 1734 CB ALA 246 8.385 13.202 65.369 1.000 25.10

ANISOU 1734 CB ALA 246 8.981 32.701 66.719 1.000 25.10

ANISOU 1735 C ALA 246 67.080 13.545 67.412 1.000 32.39 ATOM 1718 CG HIS 244 11.270 9.810 62.698 1.000 15.04 ANISOU 1718 CG HIS 244 2025 1723 1965 -178 -433 154 -272 -1236 384 -283 139 -161 -125 476 -161340 - 477-137 1939 -1248 -889 1325 ALA 246 5079 ANISOU 1735 C 4143 2632 280 428 314 ALA 246 6.876 ATOM 1736 0 14.714 67.052 1.000 32.39 ANISOU 1736 O 1247 - 66 ALA 246 4706 3748 567 3853 1737 N ALA 247 6.429 12.973 68.413 1.000 37.30 ANISOU 1737 N ALA 247 5548 5498 3126 92 640 8 3 5 1738 CA ALA 247 5.585 13.794 69.271 1.000 40.42 ANISOU 1738 CA ALA 247 5434 6048 3878 15 1313 8 5 0 ATOM 1739 C ALA 247 6.289 14.132 70.578 1.000 42.17

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						- 14/ -			
ANISOU	1739	С	ALA	247	6495	5891	3636	-823	1720 3 4 1
ATOM	1740	0	ALA		7.048	13.338	71.136		41.63
ANISOU			ALA		5811	6371	3637		
ATOM	1741		ALA		4.280			-1631	
ANISOU						13.067	69.525		47.17
			ALA		5186	9059	3676	-520	523 2683
ATOM	1742		SER		1.781	21.848	70.382		31.02
ANISOU			SER		4109	5558	2119	137	-235 -810
ATOM	1743		SER		1.214	21.932	69.052	1.000	27.01
ANISOU		CA	SER		2792	5165	2304	109	-143 - 707
ATOM	1744	CB	SER	257	0.039	22.914	68.992		28.16
ANISOU	1744	CB	SER	257	2655	4473	3572		-90 -1071
ATOM	1745	OG	SER		0.491	24.251	69.074		51.32
ANISOU		OG	SER		8516	4131	6853	-616	
ATOM	1746	C	SER		2.259	22.389	68.034		
ANISOU		C	SER	257	2537	5064			26.19
ATOM	1747		SER		3.286	22.988	235.0	-132	
ANISOU			SER		2740		68.352		31.47
ATOM						5886	3330		-689 - 639
		N	ARG		2.022	22.123	66.763		26.04
ANISOU			ARG		3257	4477	2161		-441 - 19
ATOM	1749		ARG		2.982	22.541	65.747	1.000	25.81
ANISOU			ARG	258	2606	4735	2466	73 - 33	38 -197
MOTA	1750	С	ARG		2.321	22.609	64.383	1.000	18.26
ANISOU			ARG		2374	2541	2021		-854
ATOM	1751	0	ARG	258	1.288	21.967	64.131		19.23
ANISOU		_	ARG	258	2600	2819	1888	-389	
ATOM	1752	CB	ARG		4.188	21.592	65.664		29.78
ANISOU	1752	CB	ARG		3403	5052	2861	695	-552 - 57
ATOM	1753	CG	ARG		4.246	20.784	64.384		32.64
ANISOU		CG	ARG		4358	4148	3896	146	97 - 561
ATOM		CD	ARG		5.325	19.746	64.499		30.38
ANISOU			ARG		3812	4423	3309		
ATOM		NE	ARG		6.433	19.909		-57	341 - 16
ANISOU			ARG		3990		63.581		29.43
ATOM	1756		ARG		6.453	4604	2588	-22	70 5 4 2
ANISOU						19.389	62.359		25.02
ATOM			ARG		2540	3893	3074	304	-243 1 0 4
	1757	NHI	ARG		5.456	18.677	61.835		22.88
ANISOU	175/	NHI	ARG		2105	2607	3982	359	315 289
ATOM	1758	NH2	ARG		7.523	19.593	61.617	1.000	22.03
ANISOU					2477	2775	3120	-430	
ATOM	1759		THR		2.927	23.415	63.527	1.000	20.17
ANISOU			THR		2010	3640	2013	-743	91 -1001
ATOM	1760		THR		2.485	23.505	62.138		18.33
ANISOU			\mathtt{THR}	259	1801	3043	2121		43 - 685
ATOM	1761	CB	THR	259	1.821	24.821	61.713		
ANISOU			THR		2082	3169	3576	-384	
ATOM	1762	OG1	THR	259	2.839	25.830	61.681		34.27
ANISOU	1762	OG1	THR		2181	2562	8277		-996 - 794
ATOM	1763				0.738	25.198		1 000	25.49
ANISOU	1763	CG2	тнр		4466	2233	2987		
ATOM	1764		THR	259	3.702			325	396 - 948
ANISOU						23.352	61.222		18.44
ATOM	1765		THR		2035	2822	2150	-753	
ANISOU			THR	259	4.835	23.698	61.603		24.74
ANISOU			THR		1961	5370	2069	-964	231 - 714
	1766		SER		3.420	22.867	60.026		16.29
ANISOU			SER		1971	2352	1864	-224	
ATOM	1767		SER		4.447	22.832	58.989	1.000	17.43
ANISOU			SER	260	1783	2961	1879	321	-95 -72
ATOM	1768		SER		5.224	21.514			20.17
ANISOU			SER		2306	3257	2100	762	-127 3 8 8
ATOM	1769		SER		4.416	20.392	58.698		27.09
ANISOU			SER	260	3651	2803	3839	426	217 554
		_			3 3 3 3 3	2005		740	41 J J 4

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- 148 -
        1770 C
 ATOM
                  SER
                        260 3.832
                                      23.062 57.614 1.000 14.52
 ANISOU 1770 C
                   SER
                        260 1463
                                      2165
                                              1889
                                                       83 -100 - 1
         1771 0
                   SER
                        260 2.686
                                      22.681 57.402 1.000 15.92
 ANISOU 1771 O
                   SER
                        260 1513
                                      2489
                                              2049
                                                       -93
                                                            -1 2 5 7
        1772 N
                   SER
                        261 4.617
                                      23.660 56.742 1.000 13.45
 ANISOU 1772 N
                   SER
                        261 1489
                                      1832
                                              1788
                                                       -190 -120 - 500
 ATOM
        1773 CA SER
                        261 4.294
                                      23.864 55.334 1.000 13.52
 ANISOU 1773 CA SER
                        261 1599
                                     1726
                                              1812
                                                       -204 30 - 315
        1774 C
                        261 5.209
 ATOM
                 SER
                                     22.943 54.545 1.000 12.45
 ANISOU 1774 C
                   SER
                        261 1332
                                     1887
                                              1513
                                                       -42
                                                             -240 - 161
 ATOM
        1775 0
                   SER
                        261 6.438
                                     23.072 54.662 1.000 15.07
 ANISOU 1775 O
                   SER
                        261 1344
                                     1885
                                              2497
                                                       -68
                                                             -331 - 343
 ATOM
       1776 CB SER
                        261 4.446
                                    25.330 54.943 1.000 17.76
 ANISOU 1776 CB SER
                        261 2718
                                     1625
                                              2404
                                                       -399 - 485 - 318
        1777 OG SER
 ATOM
                        261 4.428
                                    25.554 53.570 1.000 27.54
 ANISOU 1777 OG SER 261 4342
                                     3308
                                              2814
                                                       -719 -821 9 5 5
        1778 N
 ATOM
                   VAL
                        262 4.623
                                    22.045 53.782 1.000 10.90
                   VAL 262 1215
 ANISOU 1778 N
                                     1630
                                              1299
                                                       41 -135 1 9
         1779 CA VAL
                        262 5.393
                                    21.031 53.026 1.000 11.61
 ANISOU 1779 CA
                  VAL
                        262 1334
                                    1634 1442 156 -103 1
19.639 53.558 1.000 11.87
                                                            -103 1
                        262 5.026
262 1262
        1780 CB
 ATOM
                  VAL
 ANISOU 1780 CB
                                    1636 1614 9 -187 - 74
18.577 52.779 1.000 13.12
                  VAL
                                                       9 -187 - 74
        1781 CG1 VAL
ATOM
                        262 5.778
ANISOU 1781 CG1 VAL
                        262 1462
                                     1527
                                              1997
                                                      -2 185 5 1
        1782 CG2 VAL 262 5.262
ATOM
                                     19.564 55.062 1.000 17.08
ANISOU 1782 CG2 VAL
                        262 3390
                                     1494
                                              1604
                                                      -374 -245 3 9
ATOM
        1783 C
                        262 5.096
                  VAL
                                      21.149 51.543 1.000 11.18
ANISOU 1783 C
                        262 1026
                   VAL
                                      1790
                                              1431
                                                      1 -111 -138
ATOM
        1784 0
                  VAL 262 3.939
                                      20.969 51.127 1.000 12.76
ANISOU 1784 O
                  VAL
                        262 1064
                                      2137
                                              1648
                                                       -251 -84 -271
                  PHE 263 6.090 21.438 50.714 1.000 9.50
        1785 N
ATOM
ANISOU 1785 N
                   PHE 263 995 1297 1316 -6 -210 -181
ATOM
        1786 CA PHE 263 5.933 21.637 49.288 1.000 9.61
ANISOU 1786 CA PHE 263 1310
                                     1017
                                              1324
                                                       -6 -284 - 42
 ATOM
        1787 CB PHE
                        263 6.486 23.002 48.848 1.000 10.94
 ANISOU 1787 CB PHE 263 1282
                                     1055
                                              1821
                                                      -50
                                                            -253 4
 ATOM
        1788 CG PHE 263 6.150 23.399 47.418 1.000 10.35
ATOM 1788 CG PHE 263 6.150 23.399 47.418 1.000 10.35 ANISOU 1788 CG PHE 263 779 1231 1921 -58 32 340 ATOM 1789 CD1 PHE 263 6.858 22.915 46.326 1.000 9.98 ANISOU 1789 CD1 PHE 263 766 1183 1841 -26 -101 246 ATOM 1790 CD2 PHE 263 5.106 24.277 47.148 1.000 11.95 ANISOU 1790 CD2 PHE 263 1229 1261 2052 245 -29 2 ATOM 1791 CE1 PHE 263 6.530 23.229 45.019 1.000 12.49 ANISOU 1791 CE1 PHE 263 1718 1173 1857 31 -370 136 ATOM 1792 CE2 PHE 263 4.769 24.601 45.836 1.000 13.12 ANISOU 1792 CE2 PHE 263 1451 1382 2151 43 -292 353 ATOM 1793 CZ PHE 263 5.491 24.112 44.762 1.000 13.42
                                                  -26 -101 240
                                                       31 - 370 136
                                                       43 - 292 3 5 3
        1793 CZ PHE
 MOTA
                        263 5.491
                                    24.112 44.762 1.000 12.42
 ANISOU 1793 CZ PHE
                        263 1318
                                      1453
                                              1948
                                                       -138 -187 6 4 9
 MOTA
        1794 C
                   PHE
                        263 6.636
                                      20.505 48.530 1.000 8.91
 ANISOU 1794 C
                        263 1076
                   PHE
                                      1085
                                              1223
                                                       -39
                                                             -14224
 MOTA
        1795 0
                        263 7.868
                   PHE
                                      20.406 48.538 1.000 10.98
 ANISOU 1795 O
                   PHE
                        263 1098
                                      1233
                                              1842
                                                       -120 -224 -145
 MOTA
        1796 N
                   PHE
                        264 5.856
                                      19.691 47.812 1.000 9.19
 ANISOU 1796 N
                   PHE
                        264 1089
                                      1266
                                              1136
                                                       -86
                                                             -105 - 82
        1797 CA
 ATOM
                  PHE
                        264 6.386
                                      18.602 46.991 1.000 9.64
 ANISOU 1797 CA
                  PHE
                        264 1009
                                      1238
                                              1417
                                                       -56
                                                             -60 - 126
        1798 CB
 MOTA
                  PHE
                        264 5.483
                                      17.358 47.005 1.000 9.92
 ANISOU 1798 CB
                         264 1209
                   PHE
                                      1201
                                              1359
                                                       -78
                                                             17 9
 ATOM
        1799 CG
                  PHE
                         264 5.265
                                      16.673 48.336 1.000 11.22
 ANISOU 1799 CG PHE
                         264 1241
                                      1647
                                              1374
                                                       -121 38 7 7
        1800 CD1 PHE
                         264 6.292
                                      16.236 49.139 1.000 15.38
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ANISOU 1800 CD1 PHE 264 1467 2641 1734 -225 -88731801 CD2 PHE 264 3.988 16.433 48.808 1.000 16.96 ANISOU 1801 CD2 PHE 264 1425 3252 1769 -610 -79 958 1802 CE1 PHE 264 6.090 15.596 50.336 1.000 14.52 ANISOU 1802 CE1 PHE 264 1745 2417 1354 162 334 452 1803 CE2 PHE 264 3.755 15.796 50.019 1.000 18.04 ATOM ATOM 1803 CE2 PHE 264 3.755 15.796 50.019 1.000 18.04

ANISOU 1803 CE2 PHE 264 1747 3405 1704 -590 -1091008

ATOM 1804 CZ PHE 264 4.817 15.354 50.779 1.000 12.52

ANISOU 1804 CZ PHE 264 4.817 15.354 50.779 1.000 8.98

ATOM 1805 C PHE 264 1772 1536 1449 -57 227 3 3 4

ATOM 1805 C PHE 264 5.35 19.038 45.533 1.000 8.98

ANISOU 1805 C PHE 264 5.497 19.368 44.930 1.000 9.79

ANISOU 1806 O PHE 264 991 1190 1540 28 105 10 3

ATOM 1807 N LEU 265 7.758 19.031 44.999 1.000 8.43

ANISOU 1807 N LEU 265 992 884 1325 173 -180 1 5 8

ATOM 1808 CA LEU 265 992 884 1325 173 -180 1 5 8

ATOM 1808 CA LEU 265 9.309 19.964 43.328 1.000 10.10

ANISOU 1809 CB LEU 265 9.309 19.964 43.328 1.000 10.10

ANISOU 1809 CB LEU 265 9.309 19.964 43.328 1.000 10.10

ANISOU 1810 CG LEU 265 1779 1188 1469 -225 -220 2 4 8

ATOM 1810 CG LEU 265 179 1188 1469 -225 -220 2 4 8

ATOM 1811 CD1 LEU 265 1072 1009 1478 242 25 1 2 9

ATOM 1811 CD1 LEU 265 1291 1004 1811 181 -114 2 9 6

ATOM 1812 CD2 LEU 265 11.048 20.684 41.678 1.000 10.87

ANISOU 1813 C LEU 265 7.933 17.849 42.875 1.000 10.21

ANISOU 1813 C LEU 265 932 1188 1760 -6 -38 -302

ATOM 1813 C LEU 265 7.933 17.849 42.875 1.000 10.21

ANISOU 1814 O LEU 265 1388 969 1612 84 -217 1 0 7

ATOM 1815 N ARG 266 6.853 17.530 42.135 1.000 10.00

ANISOU 1815 N ARG 266 6.853 17.530 42.135 1.000 10.00 ANISOU 1803 CE2 PHE 264 1747 3405 1704 -590 -109 1 0 0 8 ANISOU 1814 O LEU 265 1388 969 1612 84 -217 107

ATOM 1815 N ARG 266 6.853 17.530 42.135 1.000 10.00

ANISOU 1815 N ARG 266 61325 1069 1404 -120 -222 1 5

ATOM 1816 CA ARG 266 6.572 16.198 41.628 1.000 10.50

ANISOU 1816 CA ARG 266 1219 1217 1554 -294 110 -210

ATOM 1817 CB ARG 266 5.208 15.675 42.124 1.000 10.56

ANISOU 1817 CB ARG 266 978 1460 1574 -168 -103 -105

ATOM 1818 CG ARG 266 4.965 15.894 43.609 1.000 11.24

ANISOU 1818 CG ARG 266 1337 1373 1563 -40 119 2 0 6

ATOM 1819 CD ARG 266 3.668 15.318 44.146 1.000 11.17

ANISOU 1819 CD ARG 266 1113 1567 1564 -17 -49 - 1 1

ATOM 1820 NE ARG 266 2.508 15.879 43.447 1.000 9.43

ANISOU 1820 NE ARG 266 1341 1157 1086 24 -100 -145

ATOM 1821 CZ ARG 266 1.236 15.509 43.657 1.000 9.83

ANISOU 1821 CZ ARG 266 1.245 1194 1294 132 -159 - 1

ATOM 1822 NH1 ARG 266 0.961 14.567 44.572 1.000 11.20

ANISOU 1823 NH2 ARG 266 1208 1240 1806 -144 -454 2 7 2

ATOM 1823 NH2 ARG 266 1460 1265 1484 191 -283 7 3

ANISOU 1823 NH2 ARG 266 6.601 16.190 40.099 1.000 10.28 1824 C ARG 266 6.601 16.190 40.099 1.000 10.28 MOTA ANISOU 1824 C ARG 266 1273 1089 1545 -200 -5 -1671825 O ARG 266 6.027 17.109 39.519 1.000 11.05 ATOM ANISOU 1825 O ARG 266 1254 1153 1793 -132 47 -6 ATOM 1826 N PRO 267 7.215 15.162 39.496 1.000 10.27 -132 47 - 64 ANISOU 1826 N PRO 267 1194 1239 1468 -33 130 3 2 1827 CD PRO 267 7.828 13.963 40.109 1.000 12.36 ATOM ANISOU 1827 CD PRO 267 1865 1132 1697 -26 -529 - ATOM 1828 CA PRO 267 7.304 15.157 38.036 1.000 10.12 -529 - 192 ANISOU 1828 CA PRO 267 1278 ATOM 1829 CB PRO 267 8.250 1095 1472 -129 38 - 185 13.986 37.767 1.000 11.83 ANISOU 1829 CB PRO 267 1489 1088 1919 -72 90 -322 ATOM 1830 CG PRO 267 8.017 13.053 38.913 1.000 10.72 ANISOU 1830 CG PRO 267 960 1356 1755 95 -257 -187

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ATOM	1831	С	PRO	267	5.977	14.929	37.344	1.000 10.86
ANISOU		С	PRO		1330	1226		
ATOM	1832	Ö					1570	-252 47 -161
			PRO	267	5.030	14.421	37.934	1.000 12.03
ANISOU		0	PRO	267	1316	1174	2080	-258 17 7 7
MOTA	1833	N	ASN	268	5.931	15.288	36.065	1.000 10.61
ANISOU	1833	N	ASN	268	1216	1146	1670	
ATOM	1834							-70 -86 -129
			ASN	268	4.810	14.949	35.198	1.000 11.20
ANISOU			ASN	268	1285	1349	1622	-167 - 43 - 229
ATOM	1835	CB	ASN	268	4.954	15.664	33.846	1.000 14.02
ANISOU	1835	CB	ASN		2160	1410	1756	
ATOM	1836							132 -316 2 3
			ASN	268	4.992	17.175	33.992	1.000 13.03
ANISOU			ASN	268	1811	1393	1747	189 -355 - 88
ATOM	1837	OD1	ASN	268	4.046	17.748	34.566	1.000 16.65
ANISOU	1837	OD1	ASN	268	1910	1744	2673	292 -1 - 159
ATOM	1838			268	6.037	17.818		
ANISOU	1070	מבוז	Y CYI				33.495	1.000 14.19
					2505	1372	1516	161 264 -172
ATOM	1839		ASN	268	4.705	13.446	34.968	1.000 10.88
ANISOU	1839	С	ASN	268	1294	1314	1526	-75 -226 - 164
ATOM	1840	0	ASN	268	5.715	12.732	34.979	1.000 11.68
ANISOU		Ō	ASN		1534	1439		
							1464	87 - 458 - 121
ATOM	1841		ALA		3.484	12.980	34.688	1.000 12.22
ANISOU		N	ALA	269	1484	1428	1732	-108 -397 - 427
MOTA	1842	CA	ALA	269	3.277	11.547	34.417	1.000 12.12
ANISOU	1842	CA	ALA	269	1432	1356	1819	-238 -29 -282
ATOM	1843		ALA		1.817			
ANISOU						11.310	34.058	1.000 12.38
			ALA	269	1439	1278	1985	-228 -183 2 9
ATOM	1844	C	ALA		4.125	10.981	33.283	1.000 11.26
ANISOU	1844	С	ALA	269	1445	1240	1592	25 - 280 - 141
ATOM	1845	0	ALA	269	4.493	9.800	33.263	1.000 12.53
ANISOU		Ō	ALA	269	1428	1249		
							2085	-110 108 -188
ATOM	1846		ASP		4.438	11.799	32.276	1.000 11.47
ANISOU			ASP	270	1701	1280	1378	-261 -341 - 300
ATOM	1847	CA	ASP	270	5.214	11.378	31.113	1.000 11.92
ANISOU	1847	CA	ASP		1826	1106	1595	19 -183 - 156
ATOM	1848	CB	ASP		4.760			
ANISOU						12.096	29.850	1.000 14.13
			ASP		1733	2038	1597	84 111 2 1 2
MOTA	1849		ASP	270	5.050	13.568	29.777	1.000 15.98
ANISOU			ASP	270	2309	1939	1823	418 -418 5 6 4
ATOM	1850	OD1	ASP	270	5.432	14.186	30.762	1.000 21.61
ANISOU	1850	OD1	ASP		4101	1797	2312	176 -515 1 6 3
ATOM	1851	002	ACD		4.880			
ANISOU	1051	002	Y O D	2/0	#.00U	14.152	28.674	1.000 24.64
					3995	3221	2145	-62 <i>-</i> 169 1 3 9 5
ATOM	1852			270	6.721	11.542	31.264	1.000 12.86
ANISOU			ASP	270	1840	1392		-398 -61 315
ATOM	1853	0	ASP		7.443	11.290		1.000 14.83
ANISOU			ASP		1813	2114	1709	
ATOM	1854							-346 -141 4 9
			PHE		7.230	11.911		1.000 11.85
ANISOU			PHE		1360	1316	1824	59 -25 7 0
ATOM	1855	CA	PHE	271	8.665	11.927		1.000 11.14
ANISOU	1855	CA	PHE		1242	1349	1641	10 230 1 6 2
ATOM	1856		PHE		8.972			
ANISOU						12.378		1.000 12.19
			PHE		1467	1444	1722	-96 -3182
ATOM	1857		PHE	271	10.385	11.992	34.597	1.000 12.77
ANISOU			PHE	271	1411	1640	1800	42 31 5 6
ATOM	1858	CD1	PHE		11.475	12.488		1.000 13.22
ANISOU	1858	CDI	DHE		1513			
ATOM						1516	1993	168 220 4 9
	1859	CD2	PRE		10.624	11.155	35.666	1.000 13.55
ANISOU	T 8 2 3	CD2	PHE		1343	1674	2131	139 84 2 5 5
ATOM	1860	CE1	PHE	271	12.779	12.178		1.000 14.26
ANISOU	1860	CE1	PHE		1432	1760	2225	-39 46 - 416
ATOM	1861			271	11.925		36 010	1 000 15 00
				411	11.343	10.806	20.019	1.000 15.88

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						- 101 -		
ANISOU	1861	CE2	PHE	271	1537	1818	2679	-263 -675 2 6 0
ATOM	1862		PHE		13.006			
						11.288		1.000 14.15
ANISOU			PHE		1166	1736	2475	7 -531 -467
ATOM	1863	C	PHE	271	9.259	10.550	32.410	1.000 11.27
ANISOU	1863	C	PHE	271	1359	1338	1585	75 271 3 4 8
ATOM	1864		PHE		8.785	9.531		
							32.920	1.000 12.97
ANISOU		0	PHE		2011	1320	1596	-85 473 279
ATOM		N	THR	272	10.261	10.498	31.541	1.000 11.95
ANISOU	1865	N	THR	272	1018	1503	2020	-214 300 -115
ATOM	1866	CA	THR		10.823	9.254	30.992	1.000 12.70
ANISOU			THR		1615	1557		
	1867						1652	132 341 146
ATOM			THR		10.679	9.281	29.450	1.000 16.79
ANISOU			THR		1814	2829	1737	-595 157 -406
\mathtt{ATOM}	1868	OG1	THR	272	9.301	9.471	29.090	1.000 18.02
ANISOU	1868	OG1	THR		1912	2921	2013	-497 -73 9 1
ATOM	1869				11.200	7.976		
ANISOU							28.856	1.000 17.02
					2144	2857	1467	-475 538 -194
ATOM	1870		THR		12.272	9.057	31.423	1.000 12.02
ANISOU			\mathtt{THR}	272	1436	1573	1559	92 603 1 3 7
ATOM	1871	0	THR		13.055	10.031	31.437	1.000 14.17
ANISOU	1871	Ο	THR		1451	1583	2351	125 602 412
ATOM	1872		PHE	273	12.625			
		•				7.837	31.828	1.000 12.34
ANISOU			PHE		1402	1585	1703	17 378 1 5 8
ATOM	1873		PHE		13.953	7.492	32.312	1.000 12.20
ANISOU	1873	CA	PHE	273	1362	1364	1909	-126 336 147
ATOM	1874	CB	PHE	273	13.951	7.514	33.861	1.000 12.37
UOSINA	1874	CB	PHE		1362	1447	1890	
ATOM	1875		PHE		12.988			
						6.528	34.491	1.000 11.65
ANISOU			PHE	273	1398	1631	1396	-367 42 -215
ATOM	1876	CD1	PHE		11.684	6.889	34.773	1.000 14.11
ANISOU				273	1531	2214	1614	-336 293 - 62
ATOM	1877	CD2	PHE	273	13.409	5.245	34.803	1.000 13.20
ANISOU					2024	1639	1352	-358 339 - 9
ATOM	1878				10.793			
ANISOU	1070	CDI	DIII			5.993	35.323	1.000 13.25
					1536	2081	1418	-98 447 4 2
ATOM	1879	CE2	PHE	273	12.530	4.329	35.327	1.000 13.39
ANISOU			PHE	273	1529	1905	1654	-224 140 283
\mathtt{ATOM}	1880	CZ	PHE	273	11.227	4.706	35.604	1.000 14.75
ANISOU	1880	CZ	PHE	273		2260	1902	-90 -186 2 7 5
ATOM	1881		PHE	273	14.423	6.135	31.795	1.000 12.45
ANISOU			PHE					
ATOM					1278	1526	1927	-120 317 - 31
	1882	0	PHE		13.645	5.311	31.291	1.000 11.95
ANISOU			PHE		1590	1580	1370	-137 226 -13
\mathtt{ATOM}	1883		SER	274	15.717	5.854	31.952	1.000 12.07
ANISOU	1883	N	SER	274	1270	1640	1677	-29 558 353
ATOM	1884	CA	SER		16.335	4.586	31.604	1.000 14.39
ANISOU			SER		1583			
ATOM	1885					1534	2349	43 707 3 8 4
_			SER		17.845	4.771	31.438	1.000 14.49
ANISOU			SER		1578	1727	2202	213 695 329
\mathtt{ATOM}	1886		SER		18.564	3.558	31.424	1.000 14.97
ANISOU	1886	OG	SER		1763	1848	2078	349 348 - 13
ATOM	1887		SER		16.100	3.505	32.666	1.000 13.12
ANISOU			SER		1670	1481		
ATOM	1888						1833	8 461 1 3 7
			SER		16.438	3.700	33.834	1.000 13.50
ANISOU			SER		1493	1518	2116	-65 119 1 5
ATOM	1889		VAL		15.533	2.359	32.271	1.000 11.90
ANISOU			VAL		1476	1618	1427	-110 490 195
ATOM	1890	CA	VAL		15.283	1.254	33.180	1.000 11.41
ANISOU			VAL		1708	1424	1204	-8 286 7 6
ATOM	1891		VAL	275	14.346	0.198	32.543	1.000 12.74
ANISOU			VAL	275	1732			
****	- U J I	<u>_</u>	AUT	4/3	7127	1300	1809	62 164 - 1 6

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ATOM 1913 CB ALA ANISOU 1913 CB ALA ATOM 1914 C ALA ANISOU 1914 C ALA ATOM 1915 O ALA ANISOU 1915 O ALA ANISOU 1916 N ARC ANISOU 1916 N ARC ANISOU 1917 CA ARC	275 2352
ATOM 1914 C ALA ANISOU 1914 C ALA ATOM 1915 O ALA ANISOU 1915 O ALA ATOM 1916 N ARO ANISOU 1916 N ARO	A 278 17.710 1.684 38.479 1.000 14.55 A 278 1972 1869 1689 -195 -255 7 9 A 278 17.894 1.770 39.683 1.000 13.80 A 278 1444 2144 1655 -250 -166 8 9 G 279 17.841 0.530 37.842 1.000 13.86 G 279 1795 1728 1742 -432 -128 1 6 9
ANISOU 1917 CA ARC ATOM 1918 CB ARC ANISOU 1918 CB ARC ANISOU 1919 CG ARC ANISOU 1919 CG ARC ATOM 1920 CD ARC ANISOU 1920 CD ARC ANISOU 1921 NE ARC ANISOU 1921 NE ARC ANISOU 1922 CZ ARC	3 279 1995 1973 2064 59 355 4 1 1 3 279 18.204 -1.922 37.648 1.000 16.83 3 279 1889 1897 2609 84 544 2 5 0 3 279 16.790 -2.323 37.291 1.000 19.63 3 279 2123 2196 3139 -63 233 9 1 3 279 16.656 -3.288 36.131 1.000 27.03 3 279 3924 3198 3150 -603 -275 - 198 3 279 17.236 -4.578 36.364 1.000 27.45 3 279 4659 2854 2915 -359 751 -789

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ANISOU 1922 CZ ARG 279 4486 3045 4948 -475 448 -2221923 NH1 ARG 279 15.424 -5.874 37.089 1.000 29.96 ANISOU 1923 NH1 ARG 279 4653 2168 4562 -103 967 -678 1924 NH2 ARG 279 17.551 -6.750 36.890 1.000 37.87 ANISOU 1924 NH2 ARG 279 4879 2436 7074 -276 3278 - 824 ARG 279 19.628 -0.519 39.150 1.000 17.48 MOTA 1925 C ARG 279 2118 ANISOU 1925 C 1653 75 -8 7 0 5 2871 1926 O ARG 279 19.916 -1.064 40.212 1.000 26.82 ATOM ANISOU 1926 O ARG 279 3764 3102 3325 -1987 -1467 1383 1927 N GLU 280 20.538 0.189 38.505 1.000 17.73 ANISOU 1927 N GLU 280 1983 2293 2459 109 609 3 7 MOTA 1928 CA GLU 280 21.899 0.317 39.026 1.000 19.66 ANISOU 1928 CA GLU 280 2049 2023 3396 125 215 737 1929 CB GLU 280 22.836 0.886 37.936 1.000 20.17 ATOM ANISOU 1929 CB GLU 280 1648 2457 3560 464 138 1099 1930 CG GLU 280 22.964 -0.149 36.818 1.000 31.79 ATOM ANISOU 1930 CG GLU 280 3477 4175 427 801 1187 - 4
ATOM 1931 CD GLU 280 23.698 0.341 35.590 1.000 39.66
ANISOU 1931 CD GLU 280 5144 5703 4221 -64 1339 - 6
ATOM 1932 OE1 GLU 280 24.466 1.327 35.685 1.000 39.65
ANISOU 1932 OE1 GLU 280 3464 5891 5710 334 574 1639
ATOM 1933 OE2 GLU 280 23.489 -0.294 34.519 1.000 41.55
ANISOU 1933 OE2 GLU 280 5257 6747 3781 2245 -184 1 0 2
ATOM 1934 C GLU 280 21.984 1.188 40.266 1.000 19.68
ANISOU 1934 C GLU 280 1488 2350 3640 -566 162 4 9 0
ATOM 1935 O GLU 280 1488 2350 3640 -566 162 4 9 0
ATOM 1935 O GLU 280 1871 3766 4123 231 -245 1 8 0
ATOM 1936 N CYS 281 20.943 1.980 40.565 1.000 18.57
ANISOU 1936 N CYS 281 1560 2609 2887 -406 -211 1 7 6
ATOM 1937 CA CYS 281 3222 2647
ATOM 1938 CB CYS 281 3222 2647
ANISOU 1938 CB CYS 281 3278 2655 3718 -426 368 -46
ATOM 1939 SG CYS 281 19.587 4.904 40.763 1.000 27.05
ANISOU 1939 SG CYS 281 19.587 4.904 40.763 1.000 27.05
ANISOU 1939 SG CYS 281 1377 1604 32.907 1.000 16.99
ANISOU 1940 C CYS 281 1377 1604 3475 109 -6-546 ANISOU 1930 CG GLU 280 3477 4175 4427 801 1187 - 4ANISOU 1940 C CYS 281 1377 1604 3475 109 -6 -546 1941 O CYS 281 19.971 3.173 43.889 1.000 17.04 ATOM CYS 281 2294 1277 2902 -204 -484 - GLY 282 19.447 1.245 42.794 1.000 15.23 ANISOU 1941 O -204 -484 - 129 1942 N ATOM ANISOU 1942 N 1597 2572 GLY 282 1617 ANISOU 1942 N GLY 282 1617 1597 2572 3 -58 - 436 ATOM 1943 CA GLY 282 18.731 0.674 43.914 1.000 15.61 ANISOU 1943 CA GLY 282 1565 1973 2394 6 -331 - 26 ATOM 1944 C GLY 282 17.246 0.519 43.727 1.000 13.75 ANISOU 1944 C GLY 282 1635 1562 2029 -270 -446 - ATOM 1945 O GLY 282 16.585 0.012 44.639 1.000 14.99 ANISOU 1945 O GLY 282 1751 1630 2313 207 -242 4 9 ATOM 1946 N PHE 283 16.744 1.009 42.582 1.000 12.65 ANISOU 1946 N PHE 283 1434 1803 1570 -200 18 - 25 ATOM 1947 CA PHE 283 15.292 0.886 42.374 1.000 11.80 3 -58 - 436 6 -331 -266 -270 -446 - 78-242 4 5 5 -200 18 - 252 1947 CA PHE 1947 CA PHE 283 15.292 0.886 42.374 1.000 11.80 ATOM ANISOU 1947 CA 1948 CB PHE MOTA ANISOU 1948 CB PHE 283 2262 972 2136 109 -187 159 283 14.906 3.351 41.757 1.000 12.63 MOTA 1949 CG PHE 283 1711 1033 2055 47 -86 9 283 13.851 3.928 42.409 1.000 13.45 283 1697 1399 2013 -166 24 - 22 ANISOU 1949 CG PHE 1950 CD1 PHE ATOM ANISOU 1950 CD1 PHE -166 24 - 229 283 16.037 4.111 41.519 1.000 13.15 1951 CD2 PHE ANISOU 1951 CD2 PHE 283 1567 1135 2295 142 -41 - 99283 13.903 5.248 42.839 1.000 15.61 283 2111 1649 2171 -202 484 -1952 CE1 PHE ANISOU 1952 CE1 PHE -202 484 -617

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ATOM 1953	CE2 E	PHE 283	16.112	5.432	41.963	1.000 12.60
ANISOU 1953	CE2 E	PHE * 283		937 206		-18 264
ATOM 1954				5.993		1.000 13.37
ANISOU 1954				865 235		
ATOM 1955				-0.534		1.000 11.23
ANISOU 1955						
ATOM 1956				974 176		-172 6 5
				-1.071	40.990	1.000 13.24
ANISOU 1956				1428		175 -120 - 361
ATOM 1957				-1.130		1.000 12.31
ANISOU 1957			1607	1333		-268 -312 8 7
ATOM 1958		ASP 284	13.589	-2.528	42.527	1.000 12.48
ANISOU 1958		ASP 284	1725	1202	1814	-148 -543 3 5 0
ATOM 1959	CB F	ASP 284		-3.156		1.000 12.67
ANISOU 1959	CB A			1145		-50 -406 1 3 5
ATOM 1960				-4.667		1.000 13.40
ANISOU 1960			2077	1171		110 -419 3 6 3
	. OD1 7			-5.246		1.000 14.98
ANISOU 1961				1094		
	OD1 1					
ANISOU 1962				-5.306		1.000 15.79
ATOM 1963			2494	1539		-330 -446 4 3 8
			12.478	-2.641		1.000 10.82
ANISOU 1963			1238	1387	1487	-205 -99 123
ATOM 1964			11.373	-3.100	41.777	1.000 12.28
ANISOU 1964			1331	1175	2159	-209 48 1 9 1
ATOM 1965		VAL 285	12.751	-2.154	40.308	1.000 11.32
ANISOU 1965		VAL 285	1204	1671	1426	-93 -48 6 1
ATOM 1966	CA 1	VAL 285	11.748	-2.062	39.260	1.000 11.45
ANISOU 1966	CA 1	VAL 285	1468	1384	1500	39 -219 - 15
ATOM 1967	CB /		12.153	-1.072		1.000 11.58
ANISOU 1967	CB 1		1412	1523	1465	-388 -428 - 8
ATOM 1968	CG1 V		12.278	0.362	38.679	1.000 15.02
ANISOU 1968	CG1 T		2209	1458	2040	-264 -442 - 32
ATOM 1969	CG2 T		13.467	-1.482	37.495	1.000 15.70
ANISOU 1969	CG2 1		1909	1443	2615	
ATOM 1970			11.424	-3.431		
ANISOU 1970			1232		38.642	1.000 10.83
ATOM 1971				1281	1602	93 -221 108
ANISOU 1971			12.267	-4.301	38.520	1.000 12.13
ATOM 1972			1214	1192	2202	-28 300 162
			10.168	-3.523	38.248	1.000 11.09
ANISOU 1972	-		1116	1608	1489	-76 967
ATOM 1973			9.558	-4.622	37.510	1.000 11.32
ANISOU 1973			1104	1479	1718	-41 -274252
ATOM 1974			8.483	-5.292		1.000 9.88
ANISOU 1974			1328	1141	1285	72 -207 7 0
ATOM 1975			7.570	-4.361	38.905	1.000 11.34
ANISOU 1975		SER 286	1391	1188	1729	147 -153 7 5
ATOM 1976	5 C S	SER 286	9.019	-4.106		1.000 10.34
ANISOU 1976			1127	1227	1575	28 -87 2 4 5
ATOM 1977			7.829	-4.112	35.869	1.000 12.62
ANISOU 1977	_		1223	2219	1353	0 -178 228
ATOM 1978			9.926	-3.622		1.000 12.45
ANISOU 1978			1414			
ATOM 1979			9.654	1664	1653	-212 3 161
ANISOU 1979				-2.900	34.099	1.000 12.59
			1622	1558	1605	-366 94 1 8 4
ATOM 1980 ANISOU 1980			10.145	-1.452		1.000 12.91
			1716	1591	1597	-373 -95 2 7
			9.452	-0.590	35.264	1.000 12.96
ANISOU 1981			1182	1848	1895	-407 -51 -170
ATOM 1982	2 CD1 :		10.229	0.708		1:000 13.34
ANISOU 1982			1644	1108	2318	-38 -124 2 2 3
ATOM 1983	3 CD2 :	LEU 287	8.006	-0.248		1.000 14.56

- 155 -

1983 CD2 LEU 287 1716 1548 2267 36 -550 3 18 1984 C LEU 287 10.319 -3.610 32.928 1.000 12.63 1984 C LEU 287 1837 1244 1710 ANISOU 1983 CD2 LEU 287 1716 36 - 550 318 LEU 287 1837 ANISCU 1984 C 1984 C LEU 287 1837 1244 1719 -233 248 3 1985 O LEU 287 11.529 -3.805 32.916 1.000 16.68 -233 248 354 ANISOU 1985 O LEU 287 1779 1998 ATOM 1986 N ASP 288 9.531 -4.045 ANISOU 1986 N ASP 288 2080 1751 2560 -292 390 -149 -4.045 31.950 1.000 13.91 1455 4 223 2 2 7 1987 CA ASP 288 10.079 -4.688 30.759 1.000 15.50 ATOM ANISOU 1987 CA ASP 288 2029 2269 1593 -122 605 153 ATOM 1988 CB ASP 288 8.979 -5.478 30.043 1.000 17.00 ANISOU 1988 CB ASP 288 2722 2125 1613 -250 362 - ATOM 1989 CG ASP 288 9.480 -6.452 29.014 1.000 19.30 ANISOU 1989 CG ASP 288 2467 2980 1885 173 243 -3 -250 362 - 2 ANISOU 2001 CG GLU 290 16.812 -2.170 27.411 1.000 27.91

ATOM 2002 CD GLU 290 3019 3161 4424 989 940 -251

ATOM 2003 OE1 GLU 290 3713 4458 4975 963 -85 -877

ANISOU 2004 OE2 GLU 290 16.336 -3.280 27.734 1.000 43.76

ANISOU 2004 OE2 GLU 290 6893 3257 6478 -30 -748598

ATOM 2005 C GLU 290 14.406 1.271 28.716 1.000 14.67

ANISOU 2005 C GLU 290 2512 1756 1308 95 142 1 0

ATOM 2005 C GLU 290 15.260 1.840 29.412 1.000 15.25

ANISOU 2006 O GLU 290 274 1969 1750 50 418 -262

ATOM 2007 N THR 291 13.232 1.814 28.437 1.000 15.72

ANISOU 2007 N THR 291 12.792 3.087 28.991 1.000 15.72

ANISOU 2008 CA THR 291 12.792 3.087 28.991 1.000 15.16

ANISOU 2008 CA THR 291 12.792 3.087 28.991 1.000 15.16

ANISOU 2009 CB THR 291 12.766 4.226 27.956 1.000 18.67

ANISOU 2009 CB THR 291 17.756 4.029 26.976 1.000 22.93

ANISOU 2010 OG1 THR 291 11.756 4.009 26.976 1.000 22.93

ANISOU 2011 CG2 THR 291 11.402 2.920 29.622 1.000 12.86

ANISOU 2012 C THR 291 11.402 2.920 29.622 1.000 12.86

ANISOU 2012 C THR 291 11.402 2.920 29.622 1.000 12.86

ANISOU 2012 C THR 291 1863 1604 1421 47 305 2 1 9 ANISOU 2012 C THR 291 1863 1604 47 305 2 1 9 1421 THR 291 10.625 2.024 29.270 1.000 16.13 THR 291 2344 1983 1804 -303 750 -ATOM 2013 0 ANISOU 2013 O -303 750 -431

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- 156 -
  MOTA
           2014 N ALA 292 11.037 3.791
                                                         30.542 1.000 12.41
                      ALA 292 1495
  ANISOU 2014 N
                                              1363
                                                                    -2 256 7 7
                                                         1859
           2015 CA ALA 292 9.746
                                              3.839
                                                         31.202 1.000 11.57
 ANISOU 2015 CA ALA 292 1362
                                              1257
                                                         1779
                                                                    -213 153 3
           2016 CB ALA 292 9.718
 MOTA
                                              2.954
                                                         32.439 1.000 12.62
 ANISOU 2016 CB ALA 292 1768
                                              1245
                                                         1784
                                                                   100
                                                                           357
           2017 C
                       ALA 292 9.385
 MOTE
                                            5.255
                                                         31.614 1.000 10.32
 ANISOU 2017 C
                       ALA 292 1317
                                              1335
                                                        1270
                                                                   -181 99 5 4
           2018 0
 MOTA
                      ALA 292 10.266 6.134 31.701 1.000 10.97
 ANISOU 2018 O ALA 292 1389
                                              1138
                                                        1641
                                                                   -146 279 104
 ATOM
           2019 N
                      THR 293 8.091
                                              5.445
                                                         31.882 1.000 12.32
           2019 N THR 293 1486 1547 1647 -314 563 -
2020 CA THR 293 7.626 6.715 32.421 1.000 12.28
 ANISOU 2019 N
 ATOM
 ANISOU 2020 CA THR 293 1717 1460
 ATOM 2021 CB THR 293 6.352 7.215 31.733 1.000 13.27 ANISOU 2021 CB THR 293 2128 1182 1730 -258 -159 -2 ATOM 2022 OG1 THR 293 5.317 6.237 31.911 1.000 13.85 ANISOU 2022 OG1 THR 293 1831 1217 2216 8 -131 7 4 ATOM 2023 CG2 THR 293 6.474 7.303 30.212 1.000 13.72 ANISOU 2023 CG2 THR 293 1791 1683 1738 -252 -56 -6
                                                        1489
                                                                   -168 337 -200
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                              293 1791 1683 1738 -252 -56 -
293 7.363 6.635 33.937 1.000 10.58
 ANISOU 2023 CG2 THR
                                                                  -252 -56 -405
           2024 C
ATOM
                       THR
ANISOU 2024 C
                       THR
                             293 1439
293 7.211
                                             1050 1533 12 447 9
5.576 34.553 1.000 10.29
MOTA
           2025 0
                       THR
                             293 1049
294 7.243
ANISOU 2025 O
                       THR
                                              1102 1758 -56 93 1 1 8
7.810 34.569 1.000 1 1.53
                                                                   -56 93 1 1 8
ATOM
           2026 N
                       PHE
ANISOU 2026 N
                             294 1794
                       PHE
                                            1093
7.939
                                                        1494 -307 306 - 66
           2027 CA PHE
ATOM
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ANISOU 2027 CA
                      PHE
                             294 1432
                                              1061
                                                         1463
                                                                   -174 125 -162
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           2028 CB PHE
ATOM
                             294 6.709
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9.658 37.770 1.000 12.77
ANISOU 2028 CB
                      PHE 294 1930
ATOM
           2029 CG
                      PHE 294 6.270
ANISOU 2029 CG PHE 294 1880
                                                        1837
           2029 CG PHE 294 1880 1136 1837 -103 178 -427 2030 CD1 PHE 294 7.123 9.462 38.839 1.000 14.73
                                             1136
ATOM
ANISOU 2030 CD1 PHE 294 1976
                                             1893
                                                        1727
                                                                   -539 161 -132
ATOM 2031 CD2 PHE 294 4.989 10.068 38.056 1.000 16.59 ANISOU 2031 CD2 PHE 294 2180 1923 2199 348 386 - 4 ATOM 2032 CE1 PHE 294 6.726 9.673 40.144 1.000 14.36 ANISOU 2032 CE1 PHE 294 1598 2028 1830 -505 280 - 1 ATOM 2033 CE2 PHE 294 4.575 10.275 39.345 1.000 16.75 ANISOU 2033 CE2 PHE 294 2214 2062 2087 692 144 - 6 ATOM 2034 CZ PHE 294 5.426 10.065 40.413 1.000 15.17 ANISOU 2034 CZ PHE 294 2040 1426 2296 327 97 - 13 ATOM 2035 C PHE 294 5.484 7.195 36.172 1.000 10.89 ANISOU 2035 C PHE 294 1401 1200 1536 -155 78 1 3 7 ATOM 2036 O PHE 294 5.325 6.425 37.125 1.000 10.67 ANISOU 2036 O PHE 294 1396 1297 1360 90 337 1 0 5 ATOM 2037 N GLN 295 4.487 7.355 35.299 1.000 10.62 ANISOU 2037 N GLN 295 1399 1187 1450 -18 88 - 24
           2031 CD2 PHE 294 4.989 10.068 38.056 1.000 16.59
ATOM
                                                                         386 -492
                                                                   -505 280 -118
                                                                         144 -602
                                                                           97 - 135
                                                                   -155 78 1 3 7
                       GLN 295 1399
 ANISOU 2037 N
                                                        1450
                                              1187
                                                                   -18
                                                                         88 - 24
                                              6.612 35.393 1.000 11.31
1205 1660 -96 120 -
7.053 34.254 1.000 11.66
1053 1953 -25 63 -14
           2038 CA GLN 295 3.217
 ATOM
 ANISOU 2038 CA GLN 295 1433
                                                                         120 - 321
 ATOM
           2039 CB
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                      GLN 295 1425
 ANISOU 2039 CB
                                              1053
                                                         1953
                                                                    -25
                                                                           63 - 141
                                              6.360
 ATOM
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                       GLN
                             295 0.951
                                                         34.200 1.000 11.05
 ANISOU 2040 CG
                       GLN 295 1573
                                              1011
                                                         1614
                                                                    -93
                                                                            -118 1 8
 ATOM
                                            6.843
           2041 CD
                       GLN 295 0.052
                                                         33.087 1.000 11.35
 ANISOU 2041 CD
                      GLN 295 1592
                                                        1395
                                              1326
                                                                   173
                                                                           57 - 13
 MOTA
           2042 OE1 GLN 295 0.349
                                              7.823 32.378 1.000 15.06
 ANISOU 2042 OE1 GLN 295 2306
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                                                        182,5 - 110
                                                                           7 3 7 9
 ATOM
           2043 NE2 GLN 295 -1.053 6.153 32.914 1.000 13.90
 ANISOU 2043 NE2 GLN
                             295 1511
                                               1757
                                                        2015
                                                                   156
                                                                         -282 2 0 8
 ATOM
          2044 C
                       GLN
                              295 3.412
                                               5.107 35.389 1.000 10.12
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						. 01. 02.
				- 157 -		
ANISOU 20	MAC	GLN 295	1154	1000	1.10.5	
	45 0			1203	1486	21 160 - 191
			2.827	4.309	36.128	1.000 11.82
ANISOU 20			1264	1542	1686	-107 41 1 3 7
ATOM 20	46 N	ASP 296	4.267	4.558	34.538	1.000 9.35
ANISOU 20	46 N		1076	1056		
	47 CA				1422	-118 -76 -275
			4.655	3.172	34.416	1.000 9 . 9 1
ANISOU 20			1241	1139	1387	56 60 - 243
ATOM 20	48 CB	ASP 296	5.699	2.852	33.347	1.000 10.26
ANISOU 20	48 CB		1315	1156	1429	113 132 - 36
ATOM 20	49 CG		5.343	2.981		
ANISOU 20					31.885	1.000 11.42
			1357	1578	1405	358 121 - 199
ATOM 20	50 OD1		4.143	2.904	31.531	1.000 13.82
ANISOU 20			1511	1744	1997	149 -209 - 62
ATOM 20	51 OD2	ASP 296	6.282	3.151	31.047	1.000 13.48
ANISOU 20			1802	1758	1564	2.000 13.48
	52 C			T170		228 364 7 3
			5.175	2.682	35.770	1.000 10.31
ANISOU 20			1416	1141	1361	16 91 - 198
	53 0	ASP 296	4.852	1.551	36.197	1.000 11.40
ANISOU 20	53 0		1428	1452	1453	-288 32 3 5
	54 N		6.004	3.484		
ANISOU 20					36.441	1.000 10.88
			1752	1144	1238	-161 11 5 5
	55 CA		6.646	3.104	37.685	1.000 11.26
ANISOU 20		TRP 297	1768	1215	1294	-217 -57 4 5
ATOM 20	56 CB	TRP 297	7.899	3.999	37.890	1.000 10.31
ANISOU 20			1387	1417	1112	-87 213 120
	57 CG		8.621			
				3.651	39.172	1.000 10.98
ANISOU 20			1456	1394	1324	164 -29 -43
ATOM 20	58 CD2	TRP 297	9.082	4.534	40.202	1.000 12.49
ANISOU 20	58 CD2	TRP 297	1255	1729	1761	75 - 298 - 197
	59 CE2		9.692	3.755	41.201	1.000 16.08
ANISOU 20	59 CF2		1860			
				2049	2202	-294 -977 4 9
ATOM 20	60 CE3		9.040	5.910	40.379	1.000 17.41
ANISOU 20			2778	1740	2096	-388 -916 - 234
ATOM 20	61 CD1	TRP 297	8.969	2.400	39.589	1.000 13.58
ANISOU 20	61 CD1		1617	1518	2025	0 -664 114
	62 NE1		9.614	2.444		
ANISOU 20					40.808	1.000 16.12
			2165	1909	2051	-22 -873 2 2 0
ATOM 20	63 CZ2		10.243	4.320	42.341	1.000 19.85
ANISOU 20			2756	2383	2404	-951 -1337 267
ATOM 20	64 CZ3	TRP 297	9.586	6.466	41.515	1.000 23.40
ANISOU 20	64 C73		4215	2030	2645	
ATOM 20	165 CH2		10.181	2030 E 670	40 40 6	
ANTCOIL 20	SEE CITA	INF 29/	10.181			
ANISOU 20	OJ CHZ		3178	2457	2537	-910 -1473 - 51
	66 C		5.700	3.138	38.882	1.000 10.39
ANISOU 20		TRP 297	1172	1448	1329	-280 -237 3 9 1
ATOM 20	67 0	TRP 297	5.574	2.159	39.639	1.000 13.52
ANISOU 20			1748	1830	1557	32 -91 7 0 3
	68 N					
			5.033	4.272	39.079	1.000 12.08
ANISOU 20			1400	1710	1480	-49 83 4 5 1
	69 CA		4.223	4.521	40.272	1.000 13.43
ANISOU 20		ILE 298	1301	2484	1317	-199 -158 - 3 3
	70 CB		4.370	5.988	40.689	1.000 16.97
ANISOU 20		ILE 298	1877			
				2908	1661	-1000 214 -630
	71 CG2		3.538	6.423	41.876	1.000 22.01
ANISOU 20	1/1 CG2		3980	3121	1263	-233 546 -339
ATOM 20	72 CG1	ILE 298	5.847	6.253	41.037	1.000 27.10
ANISOU 20	72 CG1		2588	5151	2557	-2140 -708 9 7
	73 CD1		6.365	5.522	42.266	
ANISOU 20	173 CD1					1.000 43.13
ATOM 20)74 CDI		5185	8299	2904	-3717 -3055 7 0 8
)74 C	ILE 298	3 2.772	4.116	40.131	1.000 10.94
ANISOU 20)/4 C	ILE 298	1350	1652	1156	-165 -79 9 6

			- 158 -		
ATOM 2075 O		2.137	3.844	41.155	1.000 12.67
ANISOU 2075 O		1689	1634	1493	-102 212 352
ATOM 2076 N	GLY 299	2.267	4.077	38.897	1.000 10.14
ANISOU 2076 N		1412	1057	1384	-51 -377 2 0 1
ATOM 2077 CA	GLY 299	0.866	3.822	38.695	1.000 10.72
ANISOU 2077 CA	GLY 299	1335	1084	1655	0 -229 - 206
ATOM 2078 C	GLY 299	0.049	5.054	38.369	1.000 12.05
ANISOU 2078 C	GLY 299		1293	1864	105 -292 0
ATOM 2079 O	GLY 299	0.585	6.088	37.976	1.000 13.11
ANISOU 2079 O		1917	1199	1866	174 80 - 23
ATOM 2080 N	GLY 300	-1.268	4.931	38.490	1.000 13.92
ANISOU 2080 N		1393	1531	2363	182 -410 - 223
ATOM 2081 CA	GLY 300	-2.237	5.932	38.087	1.000 14.02
ANISOU 2081 CA		1524	1471	2331	217 -563 - 336
ATOM 2082 C		-2.587	7.015	39.074	1.000 11.97
ANISOU 2082 C		940 1603		04 67	
ATOM 2083 O		-3.322	7.950	38.722	1.000 10.90
ANISOU 2083 O	GLY 300	1219	1408	1515	-37 -203 - 134
ATOM 2084 N		-2.090	6.910		1.000 11.64
ANISOU 2084 N		948 155			83 -327 165
ATOM 2085 CA		-2.195	7.915	41.323	1.000 13.39
ANISOU 2085 CA		1626	1904	1557	-191 -403 1 8 3
ATOM 2086 CB		-3.047	7.301	42.427	1.000 17.60
ANISOU 2086 CB		1391	2869	2426	-9 326 2 2 8
ATOM 2087 CG	ASN 301	-4.021	8.196	43.108	1.000 19.15
ANISOU 2087 CG	ASN 301	2549	2827	1900	805 59 3 7 7
ATOM 2088 OD:		-5.072	8.606	42.591	1.000 15.47
ANISOU 2088 OD		1258	2340	2280	-253 339 - 8
ATOM 2089 ND:		-3.661	8.510	44.367	1.000 29.28
ANISOU 2089 ND:		3585	4783	2758	1521 -850 -885
ATOM 2090 C		-0.862	8.331	41.914	1.000 11.31
ANISOU 2090 C		1436	1669	1194	1 1 -168
ATOM 2091 0		-0.033	7.456	42.221	1.000 12.03
ANISOU 2091 O		1483	1548	1542	-151 -279 8 2
ATOM 2092 N	TYR 302	-0.634	9.628	42.133	1.000 11.53
ANISOU 2092 N ATOM 2093 CA		1186	1584	1611	-61 26 1 0 2
ATOM 2093 CA ANISOU 2093 CA		0.573	10.046	42.838	1.000 11.90
ATOM 2094 CB		1260	1395	1865	5 -212 225
ANISOU 2094 CB		0.657	11.589	43.036	1.000 13.14
ATOM 2095 CG		1768 1.082	1404	1820	-273 190 181
ANISOU 2095 CG			12.287	41.750	1.000 10.88
ATOM 2096 CD:		1395 2.421	1347	1393	-321 2 -153
ANISOU 2096 CD		1385	12.439 1246	41.413	1.000 11.29
ATOM 2097 CE:		2.859	13.075	1659	-58 98 - 46
ANISOU 2097 CE		1055	1241	40.248 1732	1.000 10.60 -11 52 - 1
ATOM 2098 CD:		0.161	12.793	40.858	-11 52 - 1 1.000 11.30
		1304	1332	1656	-145 105 - 26
ATOM 2099 CE:		0.573	13.406	39.690	1.000 11.72
ANISOU 2099 CE		1013	1733	1708	-288 -138 1 6 1
ATOM 2100 CZ		1.907	13.551	39.375	1.000 10.35
ANISOU 2100 CZ		1009	1214	1709	-229 -50 -19
ATOM 2101 OH		2.284	14.153	38.202	1.000 11.82
ANISOU 2101 OH		1192	1532	1766	-8 102 1 0 4
ATOM 2102 C		0.654	9.349	44.196	1.000 12.45
ANISOU 2102 C		1517	1450	1765	-181 -202 2 1 7
ATOM 2103 O		-0.375	9.230	44.878	1.000 13.55
ANISOU 2103 O		1464	1925	1759	-339 -211 7
ATOM 2104 N		1.868	8.967	44.542	1.000 12:06
ANISOU 2104 N		1517	1653	1413	-135 -3 3 4 0
ATOM 2105 CA		2.309	8.430	45.820	1.000 11.88
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ATOM 2 ANISOU 2	165 0	1 AKG	313 4.799 313 2957 313 6.643	15.240 2293	54.659 2659	1.000 20.82 514 -234 2 6 4
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ANISOU	2166	02	AKG	312	2407	- 161 -	0505	54 255 4 2 2
ATOM	2167		AKG		2407 6.867	1765	2587 55.844	74 - 377 429
ANISOU			AKG		1997	2566	3068	1.000 20.08 -528 419 -399
ATOM	2168		AKG		7.982	14.661	55.821	1.000 17.60
ANISOU			AKG		2289	2066	2334	-314 226 -252
MOTA	2169	С3	AKG		6.272	16.080	56.872	1.000 21.69
ANISOU	2169	C3	AKG		2751	1910	3581	240 62 - 327
ATOM	2170		AKG	313		16.741	57.716	1.000 21.50
ANISOU			AKG		3246	1761	3160	199 -143 - 185
ATOM	2171		AKG		6.923	17.816	58.672	1.000 22.58
ANISOU ATOM			AKG		3122	1840	3618	755 -495 - 313
ANISOU	2172		AKG AKG		7.754	18.591	59.124	1.000 27.48
ATOM	2173		AKG		3581 5.660	2470	4389	-34 602 -1266
ANISOU			AKG		3191	17.889 2809	58.999	1.000 28.55
ATOM	2174		SO4		11.676	0.439	4846 24.942	612 -246 - 1148 1.000 40.14
ATOM	2175		SO4		11.293	0.826		1.000 40.14
ATOM	2176		SO4		12.501	-0.829	25.014	1.000 35.12
ATOM	2177		SO4		10.430	0.189		1.000 54.89
ATOM	2178		SO4		12.500	1.520	24.329	1.000 44.80
ATOM ATOM	2179		НОН	501	-6.455	10.219	44.319	1.000 14.29
ATOM	2180 2181	WO	нон нон	502	-10.520 -8.644		50.560	1.000 12.86
ATOM	2182		HOH		-8.644 -10.313	16.907	47.858 43.074	1.000 16.83
ATOM	2183		нон	505	-6.051	19.199	52.602	1.000 16.10 1.000 16.38
ATOM	2184		HOH		-6.873	24.642	47.100	1.000 20.55
ATOM	2185		HOH		10.676	-4.179	46.406	1.000 27.41
ATOM	2186		нон	508	-0.077	21.786	40.872	1.000 15.22
ATOM ATOM	2187 2188		HOH		5.761	13.656	46.041	1.000 17.40
ATOM	2189		нон нон		29.135 26.032	31.449	51.982	1.000 18.40
ATOM	2190		НОН		10.965	32.724 32.371	52.741	1.000 17.03
ATOM	2191		НОН		23.871	24.457	46.000 58.649	1.000 16.70 1.000 18.71
ATOM	2192	OW	HOH		26.353	29.063	50.326	1.000 18.71
ATOM			нон	515	23.191	33.106	53.153	1.000 20.41
ATOM	2194		нон		21.429	11.721	55.329	1.000 18.39
ATOM ATOM	2195 2196		НОН		9.122	15.567	53.585	1.000 24 .87
ATOM	2197		нон нон		27.843	17.352	53.437	1.000 27.76
ATOM	2198		HOH	520	-14.415 15.253	20.029	51.771	1.000 23.47
ATOM	2199		НОН		14.080	31.486	44.302	1.000 27.20 1.000 21.58
ATOM	2200	OW	нон		17.770	33.842		1.000 21.56
ATOM	2201		нон	523	3.671	24.673	36.173	1.000 20.95
ATOM	2202	OW	нон	524	-15.683		52.535	1.000 24.05
ATOM ATOM	2203 2204		нон	525	-5.386	20.413	39.013	1.000 26.85
ATOM	2204		нон нон	525	10.417	27.949	58.778	1.000 28.33
ATOM	2206		HOH	528	23.165 23.736	19.592 10.550	62.202	1.000 29.36
ATOM	2207		нон		-1.662	28.650	55.737 42.485	1.000 24.02
ATOM	2208		нон		-4.689	10.177	46.511	1.000 21.62
ATOM	2209		HOH	531	1.545	35.657	50.866	1.000 19.59
ATOM	2210		НОН	532	0.980	22.687	36.818	1.000 30.57
ATOM	2211		нон	533	-12.450		56.071	1.000 28.42
ATOM ATOM	2212 2213		НОН	534	-9.418	16.139	51.364	1.000 22.60
ATOM	2213	WO	нон нон		32.711	25.816	43.116	1.000 31.44
ATOM	2215	OW	HOH		27.068 13.523	24.587 11.832	55.468 51.199	1.000 23.32
ATOM	2216		HOH		8.513	16.158	35.074	1.000 10.73
MOTA	2217	OW	нон	539	0.922	2.590	35.058	
ATOM	2218		нон	540	-1.548	3.709	34.484	
ATOM	2219	OW	нон	541	11.711	16.898	30.416	1.000 17.84

ATOM

2280 OW

HOH

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HOH 11.536 32.065 1.000 17.88 6.995 52.191 1.000 17.47 MOTA 2220 OW 542 15.389 ATOM 2221 OW HOH 543 18.496 2222 OW ATOM HOH 544 19.848 22.580 35.334 1.000 17.28 ATOM 2223 OW HOH 545 -0.387 4.787 41.967 1.000 13.22 ATOM 2224 OW HOH 546 23.502 12.662 35.308 1.000 18.14 ATOM 2225 OW HOH 547 10.332 25.236 33.926 1.000 19.05 2226 OW ATOM HOH 548 21.447 20.605 34.090 1.000 17.24 2227 OW 549 8.164 ATOM HOH 7.685 27.077 1.000 25.40 2228 OW ATOM HOH 550 14.393 -5.127 40.321 1.000 15.88 MOTA 2229 OW HOH551 12.873 29.356 39.662 1.000 16.45 2230 OW ATOM HOH552 11.974 24.144 58.426 1.000 19.71 ATOM 2231 OW HOH 553 17.521 7.949 33.182 1.000 17.90 MOTA 2232 OW HOH 554 3.401 2.691 43.340 1.000 23.76 ATOM 2233 OW HOH 555 18.669 40.079 1.000 18.44 28.057 ATOM 2234 OW HOH 556 10.827 12.928 30.017 1.000 19.57 2235 OW ATOM HOH 557 20.630 16.270 66.466 1.000 20.84 MOTA 2236 OW HOH558 11.315 20.266 64.044 1.000 21.62 ATOM 2237 OW HOH 559 26.277 14.516 43.946 1.000 16.22 ATOM 2238 OW нон 560 9.616 15.488 32.365 1.000 19.40 2239 OW MOTA HOH

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29.841 43.352 1.000 43.96

602 - 3.928

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ATOM 2281 OW HOH 603 2.885 21.563 34.437 1.000 33.10 MOTA 2282 OW HOH 604 11.801 6.043 25.270 1.000 38.18 MOTA 2283 OW HOH 605 -1.019 17.197 40.472 1.000 18.48 23.349 68.110 1.000 22.54 17.197 ATOM 2284 OW HOH 606 18.382 2285 OW ATOM HOH607 -8.141 8.137 45.609 1.000 17.64 MOTA 2286 OW HOH 51.700 1.000 24.29 608 5.022 2.667 2287 OW MOTA HOH 609 17.557 10.755 33.490 1.000 21.94 ATOM 2288 OW HOH 610 11.222 1.201 49.675 1.000 20.61 2289 OW ATOM HOH 611 4.243 35.047 50.509 1.000 22.18 ATOM 2290 OW HOH 612 11.103 4.031 56.082 1.000 22.08 MOTA 2291 OW нон 613 11.366 31.522 36.791 1.000 32.32 MOTA 2292 OW HOH 614 -21.189 24.787 52.739 1.000 31.83 2293 OW MOTA HOH 615 7.847 -1.491 30.674 1.000 24.77 MOTA 2294 OW HOH 616 19.041 11.937 31.445 1.000 25.97 MOTA 2295 OW HOH 617 6.221 29.879 40.410 1.000 29.24 MOTA 2296 OW HOH 618 17.266 5.933 35.280 1.000 23.72 2297 OW ATOM 619 5.983 HOH-7.215 28.510 1.000 28.19 ATOM 2298 OW HOH 620 22.574 8.129 57.639 1.000 30.97 ATOM 2299 OW HOH 621 2.553 7.806 60.287 1.000 28.77 MOTA 2300 OW HOH 622 29.939 25.812 51.234 1.000 34.00 2301 OW ATOM HOH 623 2.205 34.823 53.632 1.000 25.88 2302 OW ATOM HOH 624 18.091 13.838 67.343 1.000 28.46 ATOM 2303 OW HOH 625 8.342 3.195 58.475 1.000 26.84 ATOM 2304 OW 626 -16.086 18.427 42.790 1.000 31.11 627 -2.098 13.445 35.620 1.000 27.48 HOH 2305 OW MOTA HOH ATOM 2306 OW 628 0.481 HOH30.471 42.834 1.000 32.55 ATOM 2307 OW HOH 629 13.368 33.845 42.899 1.000 28.70

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 ATOM 2308 OW HOH ATOM2309 OW HOH ATOM 2310 OW HOH ATOM 2311 OW HOHATOM 2312 OW HOHATOM 2313 OW HOH ATOM 2314 OW HOHATOM 2315 OW HOH ATOM 2316 OW HOH 638 6.275 39.722 1.000 25.88 34.333 ATOM 2317 OW HOH 639 2.248 19.798 56.051 1.000 26.67 ATOM 2318 OW HOH 640 -20.552 17.013 67.454 1.000 31.34 ATOM 2319 OW HOH 641 9.298 16.570 28.911 1.000 29.96 ATOM 2320 OW HOH 642 -1.732 11.113 60.074 1.000 28.13 ATOM 2321 OW HOH 643 34.157 23.604 44.657 1.000 36.36 ATOM 2322 OW HOH 644 24.298 20.199 33.576 1.000 34.90 MOTA 2323 OW HOH 645 13.803 -4.667 31.570 1.000 32.66 ATOM 2324 OW HOH 646 6.295 -2.594 29.009 1.000 34.61 647 5.623 ATOM 2325 OW HOH 37.039 49.318 1.000 28.08 MOTA 2326 OW HOH 648 -18.805 19.286 46.868 1.000 38.32 649 16.026 35.829 49.382 1.000 34.45 MOTA 2327 OW HOH 650 -12.187 28.769 45.330 1.000 27.36 ATOM 2328 OW HOH MOTA 2329 OW 651 21.344 HOH HOH 651 21.344 HOH 652 -1.848 2.125 32.240 1.000 32.24 HOH 653 -14.568 18.811 55.775 1.000 29.95 HOH 654 -8.655 26.254 38.301 1.000 32.07 5.778 55.101 1.000 27.43 MOTA 2330 OW MOTA 2331 OW MOTA 2332 OW ATOM 2333 OW MOTA 2334 OW HOH 656 16.217 14.669 25.619 1.000 33.35 ATOM 2335 OW HOH 657 28.678 14.477 38.043 1.000 30.94 2336 OW ATOM 658 -11.834 15.408 HOH 53.330 1.000 33.25 ATOM 2337 OW 659 -1.317 HOH 38.273 59.599 1.000 34.45 1.000 33.62 ATOM 2338 OW 660 8.784 HOH 13.918 28.681 MOTA 2339 OW HOH 661 -3.058 14.508 47.405 1.000 28.79 ATOM 2340 OW HOH 662 10.968 33.651 38.533 1.000 36.21 MOTA 2341 OW HOH 663 28.960 21.602 53.665 1.000 29.25

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ATOM	2342 OW	HOH	664	-10.709	26.808	39.175	1.000 42.71
\mathtt{ATOM}	2343 OW	HOH	665	17.790	7.093	55.023	1.000 30.29
ATOM	2344 OW			6.404	24.865	29.848	1.000 34.55
ATOM	2345 OW		667	-15.418	19.777	58.341	1.000 33.82
ATOM	2346 OW		668	0.000	0.000	37.259	0.330 49.90
ATOM	2347 OW		669	19.652	24.610	33.660	1.000 31.77
ATOM	2348 OW		670	17.188	9.619	29.950	1.000 29.94
ATOM	2349 OW			17.708	2.958	28.338	1.000 34.94
ATOM	2350 OW		_	-0.059	3.652	30.079	1.000 32.23
MOTA	2351 OW		673	29.037	20.923	56.153	1.000 28.52
ATOM	2352 OW		674	-15.435	31.088	53.795	1.000 35.61
ATOM	2353 OW		675	-12.846	21.220	61.856	1.000 38.79
ATOM	2354 OW		676	10.299	39.666	49.554	1.000 40.30
ATOM	2355 OW		677	-5.921	28.822	41.521	1.000 34.01
ATOM	2356 OW			6.029	39.991	46.094	1.000 42.69
ATOM	2357 OW			35.052	23.156	52.356	1.000 40.17
ATOM	2358 OW		680	-12.008	38.355	51.601	1.000 35.18
ATOM	2359 OW			3.061	13.047	53.152	1.000 35.17
ATOM	2360 OW			1.379	2.075	27.532	1.000 46.38
ATOM ATOM	2361 OW		683	-0.516	-2.480	37.686	1.000 21.77
ATOM	2362 OW 2363 OW			4.567	10.310	43.503	1.000 24.86
ATOM	2363 OW 2364 OW			19.443	5.558	61.133	1.000 36.06
ATOM	2365 OW			3.205	29.499	40.656	1.000 36.99
ATOM	2366 OW			32.498	16.774	43.447	1.000 41.18
ATOM	2367 OW		688 689	28.166	23.113	57.593	1.000 35.56
ATOM	2368 OW		-	-17.023	23.220	46.759	1.000 30.05
ATOM	2369 OW		690 691	15.567	7.782	28.910	1.000 32.51
ATOM	2370 OW		691 692	11.780	30.287	57.203	1.000 33.34
ATOM	2371 OW			24.449 26.200	12.699	32.400	1.000 34.99
111 011	23,1 000	11011	093	20.200	25.005	57.918	1.000 39.38



CLAIMS

- Deacetoxycephalosporin C synthase (DAOCS) having a structure designated by the X-ray co-ordinates of structure A or structure B herein.
- 2. DAOCS in the form of a complex with a metal, e.g. iron or lead, and optionally in the presence of a substrate and/or a substrate analogue or inhibitor, having a structure designated by the X-ray co-ordinates herein.
- DAOCS as claimed in claim 2, wherein the substrate is
 penicillin N, penicillin G, 2-oxoglutarate or dioxygen, and the inhibitor is selected from N-oxalylamino acids, pyridine-carboxylates and nitrous oxide.
- 4. Use of the three-dimensional structure of DAOCS for the modification of DAOCS or other related 2-oxoglutarate dependent enzyme.
 - 5. Use as claimed in claim 4, wherein the related 2-oxoglutarate dependent enzyme is DACS, DAOC/DACS or the oxygenase enzyme involved in the introduction of the 7α -methoxy group into cephamycin C.
 - 6. Use as claimed in claim 5 for the modification of DAOCS, DACS or DAOC/DACS such that they accept unnatural substrates more efficiently than the wild type enzymes.

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- 7. Use as claimed in claim 5 for the modification of DAOCS, DAOC/DACS such that they convert natural substrates to pharmaceuticals or useful intermediates in the preparation of pharmaceuticals.
- 8. Use as claimed in claim 6 wherein the unnatural substrates are penicillins including penicillin G, penicillin V, 6-aminopenicillanic acid, amoxycillin, or penicillins with a phenyl glycine or p-hydroxyphenyl glycine side chain.
- 9. Use as claimed in claim 6 wherein the unnatural substrate is a cephalosporin.
- 10. Use as claimed in claim 6 wherein the unnatural substrate is an amino acid, including the proteinogenic amino acids, or a peptide.
 - 11. Use as claimed in any one of claims 6-8, wherein penicillin G, penicillin V, another unnatural substrate or penicillin N is converted to a cephalosporin or exomethylene cephalosporin.
 - 12. An enzyme having significant (as herein defined) sequence similarity to DAOCS wherein the side chain binding site of penicillin N or DAOC is modified and at at least one of the following sites at least one amino acid residue is changed to another amino acid residue or is deleted: Thr72, Arg74, Arg75, Glu156, Leu158, Arg160, Arg162, Leu186, Ser187, Phe225, Phe264, Arg266, Asp301, Tyr302, Val303, Asn304; and/or at least one additional amino acid residue is inserted within the region 300-311; provided that other residues interacting with the above may be changed in order to accommodate the change in one of the above;

wherein the modifications:

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- permit the enzyme to accept unnatural substrates; and/or
- enable the enzyme to produce unnatural products; and/or
- enhance the ability of the enzyme to produce useful products.
- 5 13. An enzyme having significant (as herein defined) sequence similarity to DAOCS wherein the penicillin/cephalosporin binding site of penicillin N or DAOC is modified and at at least one of the following amino acid residues is changed or deleted: Ile88, Arg160, Arg162, Phe164, Met180, Thr190, Ile192, Phe225, Pro241, Val245, Val262, Phe264, Asn 304, Ile305, Arg306, Arg307; and/or at least one additional amino acid residue is inserted within the region 300-311; provided that other residues interacting with the above may be changed in order to accommodate the change in one of the above;

wherein the modifications:

- permit the enzyme to accept unnatural substrates; and/or
 - enable the enzyme to produce unnatural products; and/or enhance the ability of the enzyme to produce useful products.
- 14. An enzyme according to claim 12 or claim 13 which is a mutant of DAOCS or DACS or DAOC/DACS.
 - 15. An enzyme as claimed in any one of claims 12-14, wherein both the side chain and the penicillin/cephalosporin binding sites of penicillin N or DAOC are modified and at least one of the residues specified in claims 12 and 13 is changed or deleted.
 - An enzyme as claimed in any one of claims 12-15, wherein two or more complementary mutations are introduced to create or delete a binding interaction, including H-bonds, electrostatic, or hydrophobic interactions.

- 17. A gene encoding for the enzyme of any one of claims 12-16.
- 18. A micro-organism capable of expressing the gene of claim 17 under fermentation conditions.
 - 19. Use of micro-organisms of claim 18 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.
- 20. Use as claimed in claim 19 wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway including isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.
- 21. A method which comprises using the three-dimensional 15 structure of DAOCS for determining or predicting the structure of another related 2-oxoglutarate dependent enzyme or related enzyme not from the penicillin and cephalosporin biosynthesis pathway, and using the structural information so obtained for modifying the other enzyme or for designing an inhibitor for the other enzyme; wherein the said other related enzyme is 20 modified, by deletion or addition or alteration; at one or more of the sites defined in claim 12 or claim 13; or using the following information for the design of an inhibitor: Asp185, His183 and His243 act as ligands to the iron; Arg258 and Ser260 and the Fe bind the 2-oxoglutarate; Met180, 25 Phe225, Leu31 and Val245 are close to the iron binding site; Tyr33, Arg160, Arg162, Phe164, Ile192, Gln194, Leu204, Leu223, Leu215 are important for the construction of the part of the active site binding 2oxoglutarate; and Arg160 and Arg162 are important for binding an amino

acid or peptide derived substrate.

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- A method as claimed in claim 21 wherein the said other related 2-oxoglutarate dependent enzyme or related enzyme is 1-aminocylopropane-1-carboxylate oxidase, gibberellin C-20 oxidase, flavone synthase, flavanone 3β-hydroxylase, hyoscyamine 6β-hydroxylase, prolyl 4-hydroxylase, prolyl 3-hydroxylase, aspartyl hydroxylase, lysyl hydroxylase, proline hydroxylases, γ-butyrobetaine hydroxylase, enzymes in herbicide resistance mechanisms, clavaminate synthase, an oxygenase enzyme involved in the biosynthesis of carbapenems, the so called
 ethylene forming enzyme from *Pseudomonas syringe*, p-hydroxyphenylpyruvate dioxygenase, and an oxygenase enzyme involved in the oxidation of phytol in human liver peroxisomes.
- 23. A method as claimed in claim 21 or 22, wherein the said
 other related enzyme is prolyl 4-hydroxylase, prolyl 3-hydroxylase, aspartyl
 hydroxylase, or lysyl hydroxylase and the inhibitor is to be used for the
 treatment of human diseases including fibrotic diseases including liver
 cirrhosis and arthritis.
- 24. A method as claimed in claim 21 or 22, wherein the said other related enzyme is p-hydroxyphenylpyruvate dioxygenase and the inhibitor is to be used in the treatment of certain genetic disorders.
- 25. A method as claimed in claim 21 or 22, wherein the said other related enzyme is involved in herbicide resistance and the information is to be used to design new herbicides to overcome the problem of resistance.
 - 26. An enzyme as claimed in any one of claims 12 to 16, which has modifications at at least two of the said amino acid residues.

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SUBSTITUTE SHEET (RULE 26)

Fig.2.

Tyr-302

Tyr-302

Asn-304

Arg-266

er-260

H₁ = His-183

H₂ = His-243

$$\stackrel{\circ}{\longrightarrow}$$
 $\stackrel{\circ}{\longrightarrow}$ $\stackrel{\circ}{\longrightarrow}$

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My residence, 1	post office	e address and citizenship are a	s stated below next to my name	2.				
marines are fister	r perow) (of the subject matter which is	nly one name is listed below) or claimed and for which a patent /NTHASE (DAOCS) AND X-I	is sought on the inve	antian antiti-1			
(check one)		is attached hereto.						
	⊠							
I hereby state the amended by any	at I have y amendn	reviewed and understand the nent referred to above.	contents of the above identified	specification, include	ding the claims, as			
United States of	America rnational	, listed below and have also ic application having a filing da	United States Code, § 119(a)-(a international application which lentified below any foreign app te before that of the application	designated at least of lication for patent or on which priority is	one country other than the r inventor's certificate, or claimed:			
: ===				Prior	rity Claimed			
PCT/GB98/(Number		PCT (Country)	24 Dec. 1998	⊠				
	,	(Country)	(Day/Month/Year Filed)	Yes	No			
<u>⇒</u> 9727370 <u>⇒</u> (Number		United Kingdom	24 Dec. 1997					
iff (Number	,	(Country)	(Day/Month/Year Filed)	Yes	No			
9813644		United Kingdom	24 June 1998	⊠				
9727370 (Number 9813644 (Number)	(Country)	(Day/Month/Year Filed)	Yes	No			
	he benefit	under Title 35, United States	Code § 119(e) of any United S	tates provisional app	olication(s) listed below:			
(Applicat	ion Serial	No.)	(Filing Date)					
(Applicati	ion Serial	No.)	(Filing Date)					
claims of this ap paragraph of Tit	plication of plication le 35, U.S 56(a) which	lesignating the United States of is not disclosed in the prior U S.C. §112, I acknowledge the o	Code §120 of any United State of America, listed below and ins. S. or PCT international applical duty to disclose material inform date of the prior application an	sofar as the subject r tion in the manner p ation as defined in I	natter of each of the provided by the first			
(Applicati	on Serial	No.)	(Filing Date)		(Status)			

I hereby declare that all statements made herein of my own knowledge are true and that all statements made on information and belief are believed to be true; and further that these statements were made with the knowledge that willful false statements and the like so made are punishable by fine or imprisonment, or both, under Section 1001 of Title 18 of the United States Code and that such willful false statements may jeopardize the validity of the application or any patent issued thereon.

(Filing Date)

(patented, pending, abandoned)

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(Application Serial No.)

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